

Ligand-binding domain of the ultraspiracle (USP) protein

The invention relates to the spatial structure of the ligand-binding domain of the ultraspiracle protein, to the use of this structure for generating protein models of this protein in various conformations and of related proteins, and to methods of finding ligands of the ultraspiracle protein and of related proteins.

The ultraspiracle protein (termed USP hereinbelow) is the insect orthologue of the vertebrate retinoid X receptor (RXR). Like RXR, it belongs to the family of the nuclear receptors (NR). These nuclear receptors are located in the interior of the cell. They bind to responsive elements on the DNA as homo- or heterodimers and regulate the expression of genes. In order to be active they must bind specific small, frequently hydrophobic, ligands (for example steroids, retinoids, vitamin D). Nuclear receptors have a modular structure with functional domains for transactivation, DNA-binding and ligand-binding. While the DNA-binding domain of the nuclear receptors is highly conserved, the ligand-binding domains only show moderate homologies among each other. The spatial structures of various ligand-binding domains have already been determined (summary in 2) and allow an insight into the mechanism on which the activation is based, which comprises pronounced changes in the conformation of the ligand-binding domains. The binding of agonists leads to activation owing to the displacement of bound corepressors and the binding of co-activators, while the binding of antagonists prevents the interaction with the coactivator.

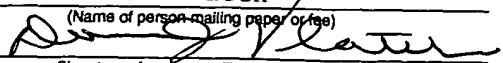
No spatial structures are available yet of insect nuclear receptors. In insects, for example the development from the larva to the adult insect is governed by nuclear receptors and involves the steroid hormone ecdysone and the isoprenoid juvenile hormone (3, 4, 5, 6). The ecdysone receptor, a nuclear receptor composed of two different subunits, EcR and USP, plays a key role in this process (7, 8, 9). It has been

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known for a long time that the hormone ecdysone (in its active form 20-hydroxy-ecdysone) acts as ligand for the EcR subunit.

The ecdysone receptor constitutes an important insecticide target. If it is activated outside the windows in the period provided for insect development, this leads to severe damage or even to the death of the insects. The insecticidal action of ecdysone agonists is based on this mechanism (10, 11). Non-steroidal ligands of the EcR subunit which act specifically on Lepidoptera are already being used commercially as insecticides (12).

USP is an orphan receptor for which no ligand is known as yet. While various authors have assumed that USP constitutes a receptor for juvenile hormones, this has never been proven by actual experiments (9). Indeed, it has been assumed that USP has no ligand at all, as this is described for some other nuclear receptors known from animals.

It was therefore an object of the present invention to provide the spatial structure of the ligand-binding domain (termed LBD hereinbelow) of the USP and to describe the possible ligand-binding pocket.

The object was achieved by providing a USP-LBD in crystalline form and by successfully carrying out the X-ray structure analysis of the crystals thus obtained.

The crystalline LBD according to the invention is preferably an LBD of the *Heliothis virescens* USP. The LBD according to the invention especially preferably has an amino acid sequence shown in SEQ ID NO: 1.

The subject-matter of the present invention is also a crystalline complex of a USP-LBD with a ligand.

The LBD according to the invention preferably has the structure coordinates defined in Table 1. The three-dimensional structure was solved and fully refined with the aid of protein crystals which are accessible to X-ray structure analysis at high resolution by means of molecular replacement. Subject-matter of the present invention is thus also the three-dimensional structure of the USP-LBD which can be determined with the aid of these structure coordinates.

A ligand-binding pocket, into which – like in the case of the other known structures of nuclear receptors – the ligands bind, has been identified in the three-dimensional structure according to the invention of the USP-LBD described herein. This is the first actual confirmation for the fact that USP has a functional ligand-binding pocket.

Subject-matter of the present invention is furthermore a USP-LBD comprising a ligand-binding pocket which is defined by the amino acids LEU230, VAL238, PRO239, PHE242, LEU249, LEU291, ILE294, MET323, LEU331, GLN338, ALA339, VAL341, PHE345, SER431, HIS434, LEU435, PHE438 and LEU440 as shown in SEQ ID NO: 2 and Table 1.

Subject-matter of the present invention is furthermore a USP-LBD comprising a ligand-binding pocket defined by the amino acids LEU230, VAL238, PRO239, PHE242, PRO245, VAL246, LEU249, CYS250, GLY253, ASN287, LEU290, LEU291, ILE294, MET323, LEU325, LEU331, SER335, ALA336, GLN338, ALA339, VAL341, ILE344, PHE345, VAL348, SER431, HIS434, LEU435, PHE438 and LEU440 as shown in SEQ ID NO: 2 and Table 1.

Subject-matter of the present invention is furthermore a USP-LBD comprising a ligand-binding pocket which is defined by the above-described amino acids and in which one or more of these amino acids are mutated. These are preferably conservative mutations, where an amino acid is exchanged for an amino acid with similar physical properties.

Such conservative substitutions encompass variations in which an amino acid is replaced by another amino acid from amongst the following group:

1. Small aliphatic residues, nonpolar residues or residues of little polarity: Ala,
5 Ser, Thr, Pro and Gly;
2. Polar, negatively charged residues and their amides: Asp, Asn, Glu and Gln;
3. Polar, positively charged residues: His, Arg and Lys;
4. Large aliphatic nonpolar residues: Met, Leu, Ile, Val and Cys; and
5. Aromatic residues: Phe, Tyr and Trp.

10

Preferred conservative substitutions can be seen from the following list:

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Original residue	Substitution
Ala	Gly, Ser
Arg	Lys
Asn	Gln, His
Asp	Glu
Cys	Ser
Gln	Asn
Glu	Asp
Gly	Ala, Pro
His	Asn, Gln
Ile	Leu, Val
Leu	Ile, Val
Lys	Arg, Gln, His
Met	Leu, Tyr, Ile
Phe	Met, Leu, Tyr
Ser	Thr
Thr	Ser
Trp	Tyr, Phe
Tyr	Trp, Phe
Val	Ile, Leu

The three-dimensional structure described herein of a USP-LBD is of great importance for the search for ligands with practical application. Such ligands can be used, for example, as insecticides with a novel mechanism of action. The ecdysone/juvenile hormone-governed development is only found in invertebrates and not in vertebrates; thus, it constitutes an insecticidal mechanism which is safe for the user and the environment.

Using the three-dimensional structure according to the invention of the USP-LBD, databases which contain the structures of a large number of compounds can be screened

with the aid of established, automated computer protocols (virtual screening). Algorithms such as FLEXX (13) or GOLD (14) are examples which can be used for virtual screening. With this procedure, compounds can be identified whose three-dimensional structure makes it possible to enter the binding pocket and to bind there, for example by forming hydrogen bonds, by hydrophobic interaction, by electrostatic interactions, by van-der-Waals interactions or by dipole interactions. The compounds identified thus can be synthesized and then used as, for example, insecticides or as effectors in expression systems (gene switch) based on the USP.

Another application of the three-dimensional structure according to the invention of the USP-LBD is the generation of new ligands. To this end, structural formulae for new ligands are generated on the computer using this structure and with the aid of established *de-novo* design programs, and these new ligands can enter the binding pocket, where they can bind, for example by forming hydrogen bonds, by hydrophobic interaction, by electrostatic interactions, by van-der-Waals interactions or by dipole interactions. Examples of *de-novo* design programs which are possible are LUDI (15), LEGEND (16) or GROW (17). Compounds generated thus can be synthesized and then also be used as, for example, insecticides or as effectors in expression systems (gene switch) based on the USP.

The three-dimensional structure according to the invention of the USP-LBD also makes it possible to predict the three-dimensional structure of a USP-LBD from other organisms by means of modelling methods. Such protein models can be used in the same manner as the three-dimensional structure solved herein. Comparison of the differences in the amino acid sequences makes it possible to predict differences in the ligand-binding pockets of various organisms. This is of use when specific ligands are searched for for specific organisms, or, conversely, when it is precisely unspecific ligands that are searched for. In addition, the three-dimensional structure according to the invention can be used for establishing protein models of other nuclear receptors with related sequences.

The present invention encompasses in particular the following subject matters and methods:

5 A computer-readable data storage medium comprising a data storage material on which the structure coordinates of an LBD according to the present invention are stored.

10 A computer-readable data storage medium in a form which makes it possible to generate a three-dimensional image of an LBD according to the present invention on a computer screen.

15 A method of generating protein models of USP-LBDs, characterized by the computer-aided generation of a three-dimensional image of an LBD according to the present invention.

A method of generating protein models of USP-LBDs in an agonistic conformation, characterized by the computer-aided generation of a three-dimensional image of an LBD according to the present invention in an agonistic conformation.

20 A method of generating protein models of nuclear receptors which have homologies with USP-LBDs, characterized by the computer-aided generation of a three-dimensional image of an LBD according to the present invention with a mutated amino acid sequence.

25 A method for generating protein models of nuclear receptors which have homologies with USP-LBDs in an agonistic conformation, characterized by the computer-aided generation of a three-dimensional image of an LBD according to the present invention with a mutated amino acid sequence in an agonistic conformation.

30 A method of finding USP ligands, characterized by the following steps:

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- (a) the computer-aided generation of a three-dimensional image of an LBD according to the present invention, and
 - (b) the computer-aided (virtual) screening of databases which contain structural data of chemical compounds for those structures which are capable of undergoing specific interactions with an LBD according to the present invention.

A method of finding USP ligands, characterized by the following steps:

10

- (a) the computer-aided generation of a three-dimensional image of an LBD according to the present invention, and
- (b) the computer-aided modelling of chemical compounds with structures which are capable of undergoing specific interactions with an LBD according to the present invention.

A method of finding USP-LBD ligands in an agonistic conformation, characterized by the following steps:

20

- (a) the computer-aided generation of a three-dimensional image of an LBD according to the present invention in an agonistic conformation, and
- (b) the computer-aided (virtual) screening of databases which contain structural data of chemical compounds for those structures which are capable of undergoing specific interactions with an LBD in an agonistic conformation.

A method of finding USP-LBD ligands in an agonistic conformation, characterized by the following steps:

30

- 5
- (a) the computer-aided generation of a three-dimensional image of an LBD according to the present invention in an agonistic conformation, and
 - (b) the computer-aided modelling of chemical compounds with structures which are capable of undergoing specific interactions with an LBD in an agonistic conformation.

10 A method of finding active compounds for crop protection, in particular chemical compounds which, owing to binding to an LBD according to the present invention, bring about the activation or inhibition of USP, with the following steps:

- 15
- (a) carrying out one of the abovementioned methods for finding USP ligands,
 - (b) synthesizing the compound(s) identified as ligands, and
 - (c) detecting the bioactivity of the compound synthesized in step (b) by transactivation assays, displacement assays or bioassays.

20 A method of finding active compounds for crop protection, in particular chemical compounds which, owing to binding to an LBD according to the present invention in an agonistic conformation, bring about the activation or inhibition of USP, with the following steps:

- 25
- (a) carrying out one of the abovementioned methods for finding USP-LBD ligands in an agonistic conformation,
 - (b) synthesizing the compound(s) identified as ligands, and
 - (c) detecting the bioactivity of the compound synthesized in step (b) by transactivation assays, displacement assays or bioassays.
- 30

A method of finding effectors for systems for the inducible expression of target genes by means of USP, with the following steps:

- 5
- (a) carrying out one of the abovementioned methods for finding USP ligands,
 - (b) synthesizing the compound(s) identified as ligands,
 - (c) applying a compound synthesized in step (b) to host cells or host organisms which contain a USP-based expression system, and
 - 10 (d) detecting an induction or inhibition of the expression system.

15 The use of an LBD according to the present invention or of a computer-readable data storage medium according to the present invention for finding active compounds for crop protection or effectors for the controlled expression of target genes in host cells or intact host organisms.

The present invention is described in greater detail with reference to the examples which follow.

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Examples

Example 1

5 Protein expression and purification

10 The *Heliothis virescens* USP-LBD (AS Val-205 to Met 466) was cloned in a pET-15b expression vector as N-terminal fusion protein with a His-tag and overexpressed in the *E. coli* strain BL21(DE3). The cells were cultured in 2x LB medium at 37°C and induced for 2 hours with 0.8 mM isopropyl-β-D-thiogalactopyranoside at 24°C. The protein extract was purified over a cobalt chelate column with subsequent gel filtration over a Superdex 200 16/60 column. The His-tag was then removed by digestion with thrombin and the protein was removed by gel filtration. A homogeneous monomeric protein species was present in the solution and was confirmed by means of SDS and native polyacrylamide gel electrophoresis and by denaturing and native electrospray ionization mass spectrometry.

Crystallization

20 Crystallization was effected by gas diffusion on hanging drops. The protein concentration employed was 3-9 mg/ml. Crystals 200 x 200 x 400 μm³ in size formed within 10 days from a solution containing 10% of polyethylene glycol (PEG) 4000, 50 mM Tris (pH 7.5), 100 mM NaCl and 5 mM dithiothreitol and which was equilibrated in the reservoir against a solution of 20% polyethylene glycol (PEG) 4000 and 100 mM Tris (pH 7.5). The crystals belong to the tetragonal P4₃22 spatial group with one monomer per asymmetric unit. The parameters of the standard cell are a=58.21 Å, b=58.21 Å, c=144.69 Å and α=β=γ=90°. The solvent content is 32%, and the B-factor estimated in the Wilson Plot is 27 Å².

Data gathering, structure determination and refining

Crystals were immersed briefly in a 10% glycerol solution and shock-frozen in liquid nitrogen. The native data set was produced with a single crystal at measuring station
5 ID14-EH2 at the ESRF (Grenoble, France). The data were processed with the aid of HKL programs (18). The crystal structure was solved by the molecular replacement method (19) by means of a partial hRXX α structure (20) as search model. A poor solution was achieved with a correlation of 24.8% and $R_{\text{free}}=54.5\%$ after refining as a rigid body. The phasing power of the model was low and required a number of
10 manual generating cycles with O (21). The wARP method (22) was used to verify the correctness of the partially-built structures. Refining was performed with CNS (23) using a maximum likelihood target function and solvent correction. Cycles of manual modelling and least-square minimization with subsequent simulated annealing and individual anisotropic B-factor refining gave rise to the final model.
15 Solvent molecules were contoured in an $F_o - F_c$ map at a surface of 3σ . The final model, refined to a resolution of 1.65 Å, comprises 246 amino acid residues, 259 water molecules and one ligand molecule. A large portion of the connecting loop between Helix H5 and the beginning of the β -pleated sheet (amino acid residues 306-315) and the C-terminal extension of H12 (amino acid residues 459-466) could not
20 be shown, owing to the poor electron density in these regions. The quality of the final model was checked with Procheck (24).

Characterization of the USP-LBD crystals by electrospray time-of-flight mass spectrometry (ESI TOF-MS) under natural conditions shows a heterogeneous mass
25 distribution around 740 ± 50 Da in addition to the peak of the pure protein (30.2 kDa). This suggested that a ligand is present which is bound in LBD. The presence of a ligand was confirmed by the electron density. Various complementary techniques were used to characterize the ligand. The ligand, which is located in the binding pocket of the USP-LBD, was characterized as a phospholipid molecule. A
30 phosphatidylglycerol or a phosphatidylethanolamine or a phosphatidylcholine would match the crystallographic data and are consistent with the results from mass

spectroscopy and chemical analysis. These amphiphilic molecules have a head group consisting of a phosphorylglycerol or a phosphorylethanolamine group and a tail of two different fatty acids which are bonded to the glycerol-3-phosphate by ester bonds. A detailed description of the ligand and its interactions with the USP-LBD residues are given in the following text.

Example 2

Architecture of the *Heliothis virescens* USP-LBD

In general, the architecture of the USP-LBD exhibits canonic NR folding with 11 α -helices (H1, H3-H12) and two short β -strands (s1-s2). This structure was compared with two other crystal structures which have essential properties of NRs and which are closely related to the *Heliothis virescens* USP: the binding pocket of agonist-bound RXR α (hRXR α /9-cis RA) and antagonist-bound mice RXR α (msRXR α /oleic acid). Superposing the USP-LBD with the structure of the holo-RXR α -LBD was carried out with the aid of a least-square fit [LSQ]. In total, the secondary structural elements of the USP-LBD are capable of reasonably good superposition by those of the holo-RXR α -LBD. The root mean square deviation (r.m.s.d.) is 1.22 Å for 183 out of 246 superposed C α atoms. Seven helices are accessible to reasonably good superposition (r.m.s.d. 1.13, 0.88, 0.57, 1.18, 0.67, 0.69, 0.75 Å for H4, H5, H7-H11). The C-terminus of H1 is curved by approximately 2 Å relative to helix H3, and its r.m.s.d. is 1.63 Å. H3, H6 and the β -pleated sheet show larger deviations. The structure of the USP-LBD demonstrates that the activation helix H12 assumes a conformation which is similar to that of the antagonist-RXR α . The antagonistic AF-2 conformation of the USP-LBD is discussed further below.

The connecting loop L1-3 of most NRs usually behaves as a highly flexible region. In the case of hRXR α , the crystal structures of both the apo and the holo conformations show substantial differences in the regions which connect helices H1 and H3. In the holo-LDB structure, L1-3 consists of an extended loop which extends

beyone the β -pleated sheet and a Ω -loop. The apo form contains an additional helix in this region which unfolds in the holo-form. During the transition from the apo-form to the holo-form, L1-3 undergoes substantial movement. In particular, the Ω -loop becomes oriented towards the opposite side of the protein centre. As has been
5 proposed on the basis of the comparison of the two structures, L1-3 might act as a molecular spring which accompanies the conformational changes which are linked to ligand binding. For the ligand-bound RAR γ -LBD, the conformation of L1-3 resembles that of the holo-RXR α . Interestingly, L1-3 for ER-LBDs follows a path other than in the case of holo-RXR α . It runs between helix H3 and the β -pleated
10 sheet, packed tightly to the protein centre.

In the case of the USP-LBD, L1-3 assumes none of the conformations which are otherwise found in the other NRs. Its course (Val-220 to Pro-239) was derived un-ambiguously from the electron density maps. Only few residues at the beginning of
15 the loop, namely Asp-222, Pro-223 and Ser-224, were treated as alanins owing to the poor electron density of the side chains. The temperature factors of these residues are therefore higher (60-64 \AA^2) than those of the other amino acids of L1-3 (on average 36 \AA^2 over L1-3). The first residues of L1-3 form a path which crosses helix H3 in the region Gln-256 to Val-262. The next residues (Glu-226 to Pro-234) form an
20 extended loop which runs along H3, and, finally, the last five residues of L1-3 (Asp-235 to Pro-239) form a loop which has substantial similarity with the Ω -loop observed in the LBDs of RXR α and RAR γ . L1-3 assumes quite a tight conformation which makes it possible to establish direct contacts with the residues of helices H3, H11 and H12 and to stabilize their actual positions. This is important in as far as
25 these helices are those structural elements which are subject to the greatest conformational changes owing to ligand binding.

The particular conformation of L1-3 is not based on crystal packing effects. In the region of the loop L1-3 of RXR α -LBD, the USP-LBD interacts with its symmetry-equivalent molecule via the β -pleated sheets. It is extremely likely that this inter-
30 action takes place since L1-3 does not already occupy this region when the protein is

in solution. If, owing to packing effects, L1-3 would be forced to swing and to move away from a conformation which is similar to the actual conformation of RXR α , several elements of the secondary structure would have to move drastically from this hypothetical conformation to their final position. It is therefore highly unlikely that this drastic reorganization of all of the LBD takes place, in particular because L1-3 lies in a region of the LBD in which L1-3 establishes very specific interactions with adjacent elements of the secondary structure.

Directly linked to loop L1-3, helix H3 differs from its counterparts in RXR α both regard to length and with regard to the position of the N- and C-terminal portion . In *Heliothis virescens* USP, H3 starts at Pro-240 and is therefore one turn longer than H3 in the ligand-bound RXR α (start at RXR α -Pro-264). The residues of H3 in the middle portion of the helix assume almost identical positions compared with the positions of the corresponding residues in the apo- and holo-RXR α -LBDs. However, both N- and C-terminal regions are curved towards the exterior of the protein centre. The N-terminal region of H3 (Pro-240 to Cys-250) is shifted substantially towards H11. It is tilted by approximately 24° in comparison with the same region in the holo-RXR α (approx. 7.2 Å between USP-Pro-245 and holo-RXR α -Pro-264). This position lies between those of the N-terminal regions in the apo-RXR α and the holo-RXR α -LBD structure. The outwardly curved C terminus of H3 (by approx. 10°) has effects on the arrangement of the adjacent loops L3-4 and L8-9. Loop L3-4, which is part of the signature region of NRs, is shifted laterally by approximately 1.8 Å and curved towards L8-9, while loop L8-9 itself is shifted outwardly by approximately 1.5 Å.

Example 3

The ligand-binding pocket

The ligand-binding pocket of *Heliothis virescens* USP is formed by residues of loop L1-3, helices H3, H5, H6 and H7, the β -pleated sheet and loop L11-12. As described

above, the N-terminal portion of helix H3 is markedly shifted outwardly compared with its opposite number in RXR α . Two other secondary structures which contribute to the binding pocket also differ from those in RXR α : 1) Helix 6 has moved inwardly by approximately 1.9 Å, and 2) the curvature of the β -pleated sheet points towards H1. The shift of the three structural elements which this entails lead to a widening of the ligand-binding pocket compared with that of the RXR α -LBD. The edge of the binding pocket is formed by the Ω -loop of L1-3, the N terminus of H3 and H6, while in the case of RXR α the opening of the pocket is formed by loop L11-12 and H6. At its opening, the binding pocket is approximately 13.5 Å wide (distance between Lys-241 in H3 and Gln-338 in H6). This opening is much wider than in the case of RXR α (7.1 Å from Pro-264 in H3 to Ala-340 in H6). The topology of the ligand-binding pocket is relatively unusual with a gap between H3 and H6. In RXR α and other NRs, this region forms fixed contacts with the connecting loop L1-3. The volume of the cavity of the USP-LBD achieves that of the hRXR α -LBD by a factor of 2.5 (1256 Å³ in the case of USP compared with 489 Å³ in the case of hRXR α).

Example 4

The putative ligand of USP in the crystal structure

Unexpectedly, the ligand-binding pocket of *Heliothis virescens* USP contains a molecule which was copurified and cocrystallized together with the USP-LBD. The fit of the electron density agrees well with the characterization of the molecules by mass spectroscopy and analytical chemistry. Similarly, recent crystallographic studies of the heterodimeric RAR α /RXR α -LBD show an *E.coli*-endogenous oleic acid (C18) or a similar compound (stearic (C18) or palmitic (C16) acid) in the RXR α subunit. Even though this molecule is not the natural ligand of vertebrate NR, it induces and stabilizes an antagonistic AF-2 conformation which in all probability is very similar to the actual antagonist-bound RXR α .

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In the present case, the best fit of the electron density was assumed with the assumption of a phospholipid whose first tail consists of a fatty acid with a length of 18 carbon atoms at C1 and a second chain at C2 which is 16 carbon atoms in length. The longer fatty acid of the two has a relatively twisted shape with two largish peaks, while the other fatty acid assumes a more normal form within the pocket. The tail of the phospholipid is hidden within the ligand-binding pocket. The glycerol moiety and the two fatty acids form van-der-Waals contacts with the residues in L1-3 (Leu-230, Val-238), H3 (Phe-242, Leu-249), H5 (Leu-291), L6-7 (Ala-339), H7 (Phe-345), H11 (Ser-431, His-434, Phe-438) and L11-12 (Leu-440). The head group of the phospholipid is positioned at the front at the opening of the pocket between H3 and H6. A strong hydrogen bond with Gln-338 (H6) is formed by the carbonyl group of the phosphorylglycerol in the case of phosphatidylglycerol and by the amino group of the ethanolamine in the case of phosphatidylethanolamine. In addition, an oxygen of the phosphate group is bound to a residue L1-3 (C γ of Pro-239) by a hydrogen bridge.

It is assumed that the phospholipid found herein constitutes no natural USP ligands. However, it is shown unambiguously that USP ligands exist.

The residues which interact with the ligands are highly conserved within lepidopteran USPs, with the exception of Ser-431, which is replaced by a cysteine in msUSP. In contrast, among the 16 residues of the RXR α -LBD which interact with 9-*cis* RA, only 3 of the corresponding USP residues interact with the phospholipid (Leu-249, Ser-431 and His-434). The reason for this behaviour is mainly the different position of the ligands in the corresponding pockets. The 9-*cis* RA is very deep within the pocket, where its carboxylate group forms a salt bridge to Arg-316 of helix H5 of the hRXR α . In contrast, the phospholipid does not penetrate far into the inside of the pocket. For example the tail of the longer fatty acid lies approximately at atom C9 of 9-*cis* RA in hRXR α -LBD, while the tail of the other fatty acid extends almost to the β -ionone ring of 9-*cis* RA. As a consequence, Arg-297 does not participate in the anchorage of the ligand, as is observed in the case of the agonistic RXR α -, RAR γ -

and other NR-LBDs. Nevertheless, it assumes almost the same position as Arg-316 of the holo-RXR α and not the position of the apo-RXR α conformation, which is exposed to the solvent. Instead of interacting with the ligand, Arg-297 forms hydrogen bonds with the backbone carbonyl group of Leu-325 (β -pleated sheet) and participates in a hydrogen bond network with Leu-290 (H5) and the side chain of Gln-256 (H3), with participation of water. In particular, two water molecules which are positioned spatially approximately at the two oxygen atoms of the carboxylate group of 9-*cis* RA participate in these interactions.

Example 5

The antagonistic conformation of the USP-LBD

The AF-2 domain in the structure of the USP-LBD exhibits an antagonistic conformation generated by the ligands in the ligand-binding pocket. H12 assumes the same conformation which has been found in the case of other antagonist-bound nuclear receptors such as RXR α /oleic acid, RAR α /BMS614 and ER. In all these cases, it is observed that the groove in which H12 is positioned corresponds to the binding site for the helical nuclear receptor box of nuclear receptor coactivators. This helical nuclear receptor box is distinguished by the consensus sequence LXXLL, as has been shown for the ligand-binding domain of PPAR γ , TR β and ER α . In the case of the *Heliothis virescens* USP, Ile-450, Ala-453 and Leu-454 of H12 are approximately in the same position as the first, second and third leucin residue of the LXXLL binding motif (IXXAL instead of LXXLL). As in other antagonistic conformations of nuclear receptors, H12 is packed into a groove of residues of H3 and H4 and of L3-4 (Val-261, Arg-265, Met-275, Glu-276, Ile-279, Ile-282, Lys-283). However, in the case of the USP-LBD, L1-3 is also involved in the groove topology and, with the residues Phe-227, Gln-228 and Phe-229, has van-der-Waals contacts with H12.

The length of H12 in the USP-LBD is identical to that of H12 in the antagonist-bound form of the RXR α -LBD. However, the structural principle which has been observed in another case of an antagonistic conformation of a nuclear receptor ligand-binding pocket is not found in its entirety in the case of the USP-LBD. Indeed, it has
5 been found there that H11 coils up and thus permits H12 to bind to the binding groove of the nuclear receptor coactivator binding motif LXXLL. H11 is located in the extension of H10 and superposes very readily with H11 in the holo-RXR α -LBD structure, with the exception that the H11 of the USP-LBD is shorter by two residues. This is followed by a region 6 residues in length which connects H11 and H12 (His-
10 439 to Thr-444). These amino acids of loop L11-12 span, in an extended conformation, a strand 12 Å in length. The C terminus of H11 contains three phenylalanines which are also found in RXR α . In apo-RXR α , the first two phenylalanines point towards the hydrophobic ligand-binding pocket while the third phenylalanine faces the solvent. In the agonist-bound form, the phenylalanines swap roles. In the
15 USP-LBD, the situation is similar to the agonist-bound form of the RXR α -LBD: Phe-436 and Phe-437 face the solvent, while Phe-438 contributes to the ligand-binding pocket. In comparison with its counterpart in RXR α , the side chain of Phe-438 is rotated slightly and touches the ligand at the level of its shorter fatty acid. In the antagonist-bound form of RXR α , the first residue of the phenylalanine triplet
20 corresponds to the end of H11. This residue is in approximately the position of the C- α atom of Phe-437. In the ligand-binding pocket, the two other phenylalanine residues, which are already part of L11-12, are orientated inwardly towards the inside of the protein. In a superposition of the *Heliothis virescens* USP and the antagonist-bound RXR α -LBD, these two residues collide with the phospholipid ligands.

Example 6

The connecting region L1-3 interacts with H3 and L11-12 and prevents an agonistic conformation

5

The binding of the phospholipid in the ligand-binding pocket of the USP-LBD probably generates important structural rearrangements in the USP-LBD. The comparison with apo- and holo-RXR α -LBD structures allows the assumption that in the USP-LBD, too, the molecular mechanisms which bring about the ligand-bound LBD conformation comprise the displacement of H3 and H11. However, in contrast to all other nuclear receptor LBDs known to date, the structural element L1-3 plays an essential role in the *Heliothis virescens* USP.

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Loop L1-3 interacts with H3, H11, L11-12 and H12. These structural elements are most effectively by the ligand binding. L1-3 stabilizes the N-terminus of H3 via a hydrogen bridge network with Arg-243 and Asn-254 of H3. The guanidinium moiety of the Arg-243 is anchored to the backbone carbonyls of Gly-233, Ser-236 and Val-238 by strong hydrogen bridges (distances 2.61, 2.97 and 2.78 Å, respectively) and shows a van-der-Waals contact with the side chain of Val-232. In addition, the backbone amide group of the Arg-243 is bound to the carbonyl group of Pro-239 (3.20 Å) by a hydrogen bond. The side chain of Asn-254 forms hydrogen bonds with the carbonyl group of Leu-230 (2.83 Å), to the amide group of Phe-229 (3.10 Å) and, via a water molecule, to the side chain of Gln-228. Moreover, it is in van-der-Waals contact with the carbonyl group of Phe-227. The backbone carbonyl group of Asn-254 forms a strong hydrogen bridge to the side chain of Glu-226 (2.74 Å).

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L1-3 (Gln-228 to Arg-231, Asp-235 and Ser-236) is also in contact with N-terminal region of H11 and with L11-12. The backbone carbonyl group of Gln-228 forms a hydrogen bond with Ala-442 (3.20 Å), and the backbone carbonyl group of Phe-229 forms a strong hydrogen bridge with the amide group of Ala-442 (2.88 Å). In addition, Arg-231 stabilizes the loop L11-12 by means of strong interactions: the

backbone amide group forms a strong hydrogen bond with the carbonyl group of Leu-440 (2.90 Å), while the side chain forms a strong hydrogen bond with the carbonyl group of His-439 (3.00 Å) and shows van-der-Waals contacts with Val-441 and Ala-442. Other interactions concern the backbone carbonyl of Asp-235 with the side chain of His-439 and a water-mediated interaction with Val-441. The hydroxyl group of Ser-236 forms a van-der-Waals contact with the side chain of Leu-440.

It is important to state that a high degree of sequence conservation exists in all residues which participate in the interaction of L1-3 with H3 and with L11-12. The main interaction partners of H3, Arg-243 and Asn-254, are conserved strictly in all lepidopteran USPs. Likewise all interaction partners in L1-3 (Glu-226, Phe-227, Gln-228, Phe-229, Leu-230, Val-232, Gly-233, Ser-236, Val-238, Pro-239) are conserved strictly in all lepidopteran USPs, with the exception of Phe-227 and Phe-229, which are replaced by leucine and isoleucine in the *Bombyx mori* USP. In the case of the interactions of L1-3 with L11-12, too, the residues involved (L1-3: Gln-228 to Arg-231, Asp-235 and Ser-236; L11-12: His-439 to Ala-442) are conserved strictly in all lepidopteran USPs, with the exception of Phe-229 and Asp-235. This strongly suggests that interaction patterns of L1-3 with H3 and of L1-3 with L11-12 are similar in all lepidopteran USPs.

In the superposition of *Heliothis virescens* USP with the holo-RXR α -LBDs, it can be observed that some residues from L1-3 are approximately in the same position in the *Heliothis virescens* USP (Asn-237, Ser-236 and Phe-229), such as residues from L11-12 of holo-RXR α (Asp-444, Thr-445 and Phe-450). This comparison permits the informative conclusion that L1-3 in its actual conformation excludes the existence of an agonistic conformation since this would be hindered at loop L11-12. In any case, this is no crystallization artefact and reflects the particular role of this structural element in the lepidopteran USPs.

The sterical hindering of the agonistic position of H12 here is a constitutive component of the receptor structure and not the consequence of the bulky shape of

the ligand, as is the case in other nuclear receptor LBDs which are occupied by fully antagonistic ligands.

5 It can be predicted that ligand binding of agonists generates a change in the conformation of the USP-LBD, which makes L1-3, H12 and the other LBD residues which have been described jump into an antagonistic position.

In any case, this is not a crystallization artefact and constitutes the particular role of this structural element in the lepidopteran USPs.

10

Example 7

Agonistic conformation of the *Heliothis virescens* USP-LBD by homology modelling, based on the RXR α /9-cis-RA complex

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In order to generate a 3D model of the *Heliothis virescens* USP-LBD, the lacking residues of the loop between helices H1 and H3 (L1-3) were complemented from the hRXR α crystal structure in such a way that a continuous backbone is formed. The resulting structure is the experimental hRXR α reference model.

20

Two hRXR α monomers were observed in the hRXR α standard cell, and the L1-3 region was poorly resolved in each of these monomers. Superposition of the two structures, which had been refined independently of one another, led to a suggestion as to where this loop should be modelled. A complete 3D model of hRXR α based on
25 crystal structure and in which the residues in L1-3 are completed was built. The hydrogen atoms were completed with the aid of the Hgenerate option of the Charmm program.

30 The L1-3 region was relaxed by Powell minimization of the Charmm program (1000 optimization steps, dielectric constant : 4, gradient tolerance : 10^{-6} , step width 0.02, cutoff for non-binding interactions: 15 Å).

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This optimized structure was used as template for the homology model of the *Heliothis virescens* USP-LBD.

- 5 The amino acid sequences of the *Heliothis virescens* USP-LBD and of hRXR α were assigned in accordance with Table 2.

10 With the aid of the software package Modeller and its standard settings, a 3D model was built with the aid of the assignment. The USP-LBD sequence shows a few insertions in loop 1-3 and in the loop before the first β -pleated sheet. In order to establish meaningful conformations for these two regions, the option lego-loop of the software package O was used. The USP model structure was subsequently subjected to Powell minimization (2000 optimization steps, dielectric constant: 4, gradient tolerance: 10^{-6} , step width 0.02, cutoff for non-binding interactions: 15 Å). The
15 quality of the structure thus obtained is analyzed with the program PROCHECK. Accordingly, 97% of the residues are in permitted regions and less than 2% of the residues are in prohibited regions. The latter are in the above-described modified regions.

20 **Example 8**

Comparison between the agonistic USP-LBD structure obtained from the hRXR α /9-cis RA complex and the USP-LBD crystal structure

- 25 The largest differences between these two structures are in the position of the activation helix (H12) and the path of the loop between the helices H1 and H3. The activation helix H12 is located in the experimental structure in the antagonistic position, while in the model structure it assumes an agonistic conformation which closes the ligand-binding niche. In the experimental structure, the loop L1-3 lies
30 above the helix H3 and stabilizes the antagonistic position of H12 by hydrophobic contact. In contrast, this loop lies at a considerable distance from the central AFS-AD

helix in the agonistic homology model. Loop L1-3 is separated from helix H3 by the β -pleated sheet.

Moreover, the size of the ligand-binding niche differs substantially between the two structures. The presence of the large fatty acid residue in the USP-LBD crystal structure causes a great cavity by shifting helices H3, H6 and H11. In the USP agonistic conformation, these helices are packed densely and produce a smaller ligand-binding niche.

10 The regions of the C-terminal ends of H3, H4, H5, H8 and H9 are rigid and capable
of very good superposition in the two structures. In contrast, loop L1-3 and the C-
termini of H3, H6 and H11 in the two structures are displaced relative to each other.
These segments form the most mobile region of the ligand-binding domain of nuclear
receptors. This movement is probably specific for each receptor and the ligand-
15 generated displacement.

Information on the sequence listing

SEQ ID NO: 1 shows the amino acid sequence of the *Heliothis virescens* USP-LBD.

SEQ ID NO: 2 shows the amino acid sequence of the *Heliothis virescens* USP.

Information on the Tables

Table 1 shows the structure coordinates of the LBD of the *Heliothis virescens* USP.

- 5 Table 2 shows the amino acid sequence assignment for hRXR α and USP of *Heliothis virescens* and of further nuclear receptor LBDs for generating a homology model of the agonistic USP conformation.

Table 1

10 REMARK coordinates from restrained individual B-factor refinement
 REMARK refinement resolution: 20.0 - 1.65 Å
 REMARK starting $r = 0.2151$ free_ $r = 0.2506$
 REMARK final $r = 0.2112$ free_ $r = 0.2459$
 REMARK B rmsd for bonded mainchain atoms= 1.437 target= 1.5
 15 REMARK B rmsd for bonded sidechain atoms= 2.272 target= 2.0
 REMARK B rmsd for angle mainchain atoms= 2.299 target= 2.0
 REMARK B rmsd for angle sidechain atoms= 3.310 target= 2.5
 REMARK rweight= 0.1000 (with wa= 1.12122)
 REMARK target= mlf steps= 30
 20 REMARK sg= P4(3)22 a= 58.211 b= 58.211 c= 144.687 alpha= 90 beta= 90 gamma= 90
 REMARK parameter file 1 : CNS_TOPPAR:protein_rep.param
 REMARK parameter file 2 : CNS_TOPPAR:water_rep.param
 REMARK parameter file 3 : eph.par
 REMARK molecular structure file: alternate.mtf
 25 REMARK input coordinates: anneal_2.pdb
 REMARK reflection file= /home/billas/USP/SCALE0400/merge1A65/usp_20a1a65.10.cv
 REMARK ncs= none
 REMARK B-correction resolution: 6.0 - 1.65
 REMARK initial B-factor correction applied to fobs :
 30 REMARK B11= -1.985 B22= -1.985 B33= 3.970
 REMARK B12= 0.000 B13= 0.000 B23= 0.000
 REMARK B-factor correction applied to coordinate array B: -0.193
 REMARK bulk solvent: density level= 0.33501 e/Å³, B-factor= 48.7849 Å²
 REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
 35 REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected

REMARK theoretical total number of refl. in resol. range: 30842 (100.0 %)
REMARK number of unobserved reflections (no entry or |F|=0): 1417 (4.6 %)
REMARK number of reflections rejected: 0 (0.0 %)
REMARK total number of reflections used: 29425 (95.4 %)
5 REMARK number of reflections in working set: 26453 (85.8 %)
REMARK number of reflections in test set: 2972 (9.6 %)
CRYST1 58.211 58.211 144.687 90.00 90.00 90.00 P 43 2 2
REMARK FILENAME="/home/billas/LUC/13cns/bind_2.pdb"
REMARK DATE: 4-Jun-00 14:33:10 created by user: billas

10 REMARK VERSION:1.0

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15	ATOM	5	CA	ALA	203	16.347	28.703	40.490	1.00	66.40
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20	ATOM	10	O	ALA	204	12.259	27.413	40.890	1.00	65.54
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ATOM	18	CB	GLN	206	11.198	26.298	44.472	1.00	58.55	
ATOM	19	CG	GLN	206	11.976	25.062	44.863	1.00	60.08	
30	ATOM	20	CD	GLN	206	12.831	24.542	43.712	1.00	61.69
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5	ATOM	31	OE2	GLU	207	5.235	23.125	42.043	1.00	58.53
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	ATOM	33	O	GLU	207	9.419	21.945	45.089	1.00	44.54
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10	ATOM	36	CB	LEU	208	6.204	21.323	47.752	1.00	36.20
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	ATOM	38	CD1	LEU	208	7.495	21.026	49.867	1.00	32.61
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15	ATOM	41	O	LEU	208	6.443	19.122	45.919	1.00	38.80
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25	ATOM	51	CG2	ILE	210	12.017	12.667	47.387	1.00	37.65
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	ATOM	53	CD1	ILE	210	9.239	13.004	48.447	1.00	35.19
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	ATOM	105	SD	MET	216	14.067	22.656	50.591	1.00	29.63
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10	ATOM	108	O	MET	216	18.955	20.998	52.755	1.00	32.43
	ATOM	109	N	GLU	217	18.381	18.982	51.923	1.00	34.02
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30	ATOM	128	CD1	LEU	219	21.879	22.395	49.219	1.00	51.07
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	ATOM	135	CG1 VAL	220	26.774	23.341	56.456	1.00	51.60
	ATOM	136	CG2 VAL	220	26.142	21.426	54.965	1.00	50.84
	ATOM	137	C VAL	220	25.030	25.106	54.770	1.00	55.56
	ATOM	138	O VAL	220	25.929	25.613	54.097	1.00	56.16
5	ATOM	139	N ALA	221	24.147	25.823	55.450	1.00	57.83
	ATOM	140	CA ALA	221	24.190	27.278	55.428	1.00	60.51
	ATOM	141	CB ALA	221	22.782	27.845	55.601	1.00	60.73
	ATOM	142	C ALA	221	25.108	27.838	56.499	1.00	61.87
	ATOM	143	O ALA	221	25.475	27.143	57.452	1.00	62.13
10	ATOM	144	N ALA	222	25.490	29.100	56.326	1.00	62.85
	ATOM	145	CA ALA	222	26.345	29.756	57.295	1.00	63.37
	ATOM	146	CB ALA	222	26.612	31.196	56.871	1.00	63.59
	ATOM	147	C ALA	222	25.564	29.719	58.601	1.00	63.51
	ATOM	148	O ALA	222	24.422	30.176	58.659	1.00	63.95
15	ATOM	149	N ALA	223	26.173	29.150	59.636	1.00	63.63
	ATOM	150	CA ALA	223	25.532	29.044	60.939	1.00	63.10
	ATOM	151	CB ALA	223	26.558	28.627	61.984	1.00	63.64
	ATOM	152	C ALA	223	24.874	30.365	61.339	1.00	62.58
	ATOM	153	O ALA	223	25.557	31.333	61.678	1.00	63.33
20	ATOM	154	N ALA	224	23.544	30.399	61.290	1.00	61.31
	ATOM	155	CA ALA	224	22.789	31.599	61.644	1.00	59.25
	ATOM	156	CB ALA	224	21.323	31.440	61.220	1.00	58.51
	ATOM	157	C ALA	224	22.878	31.880	63.143	1.00	58.07
	ATOM	158	O ALA	224	22.988	30.943	63.939	1.00	58.18
25	ATOM	159	N GLU	225	22.844	33.159	63.528	1.00	56.07
	ATOM	160	CA GLU	225	22.909	33.507	64.950	1.00	54.05
	ATOM	161	CB GLU	225	22.498	34.969	65.221	1.00	54.53
	ATOM	162	CG GLU	225	22.700	35.401	66.703	1.00	55.83
	ATOM	163	CD GLU	225	21.439	35.872	67.407	1.00	56.62
30	ATOM	164	OE1 GLU	225	21.407	35.822	68.663	1.00	57.35
	ATOM	165	OE2 GLU	225	20.464	36.314	66.743	1.00	57.42
	ATOM	166	C GLU	225	21.901	32.594	65.611	1.00	52.71
	ATOM	167	O GLU	225	20.737	32.557	65.201	1.00	52.66
	ATOM	168	N GLU	226	22.334	31.840	66.612	1.00	50.26
35	ATOM	169	CA GLU	226	21.391	30.960	67.256	1.00	47.92
	ATOM	170	CB GLU	226	21.858	29.513	67.196	1.00	49.61

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	ATOM	171	CG	GLU	226	20.778	28.525	67.641	1.00	49.78
	ATOM	172	CD	GLU	226	19.333	28.959	67.359	1.00	51.91
	ATOM	173	OE1	GLU	226	18.452	28.312	67.956	1.00	50.08
	ATOM	174	OE2	GLU	226	19.039	29.909	66.543	1.00	51.77
5	ATOM	175	C	GLU	226	21.015	31.344	68.670	1.00	46.28
	ATOM	176	O	GLU	226	21.839	31.794	69.476	1.00	47.17
	ATOM	177	N	PHE	227	19.733	31.155	68.942	1.00	41.52
	ATOM	178	CA	PHE	227	19.138	31.503	70.206	1.00	38.73
	ATOM	179	CB	PHE	227	17.723	32.022	69.963	1.00	40.03
10	ATOM	180	CG	PHE	227	17.640	33.061	68.876	1.00	40.91
	ATOM	181	CD1	PHE	227	17.775	32.703	67.542	1.00	40.72
	ATOM	182	CD2	PHE	227	17.464	34.402	69.192	1.00	42.62
	ATOM	183	CE1	PHE	227	17.739	33.661	66.535	1.00	42.04
	ATOM	184	CE2	PHE	227	17.426	35.374	68.188	1.00	42.27
15	ATOM	185	CZ	PHE	227	17.564	34.996	66.857	1.00	42.02
	ATOM	186	C	PHE	227	19.119	30.339	71.174	1.00	34.83
	ATOM	187	O	PHE	227	19.218	29.178	70.778	1.00	34.52
	ATOM	188	N	GLN	228	18.982	30.687	72.445	1.00	33.69
	ATOM	189	CA	GLN	228	18.979	29.735	73.540	1.00	32.01
20	ATOM	190	CB	GLN	228	19.290	30.468	74.847	1.00	34.80
	ATOM	191	CG	GLN	228	20.680	31.080	74.935	1.00	39.39
	ATOM	192	CD	GLN	228	21.768	30.029	74.916	1.00	40.63
	ATOM	193	OE1	GLN	228	22.117	29.504	73.860	1.00	44.27
	ATOM	194	NE2	GLN	228	22.301	29.706	76.093	1.00	42.65
25	ATOM	195	C	GLN	228	17.678	28.974	73.736	1.00	28.92
	ATOM	196	O	GLN	228	17.035	29.174	74.750	1.00	28.29
	ATOM	197	N	PHE	229	17.283	28.120	72.794	1.00	28.04
	ATOM	198	CA	PHE	229	16.056	27.340	72.996	1.00	25.30
	ATOM	199	CB	PHE	229	15.767	26.411	71.821	1.00	27.02
30	ATOM	200	CG	PHE	229	15.066	27.055	70.680	1.00	28.71
	ATOM	201	CD1	PHE	229	15.599	28.170	70.052	1.00	28.96
	ATOM	202	CD2	PHE	229	13.903	26.480	70.173	1.00	30.61
	ATOM	203	CE1	PHE	229	14.991	28.708	68.918	1.00	29.32
	ATOM	204	CE2	PHE	229	13.284	26.998	69.046	1.00	31.44
35	ATOM	205	CZ	PHE	229	13.829	28.117	68.412	1.00	31.43
	ATOM	206	C	PHE	229	16.276	26.434	74.195	1.00	23.81

	ATOM	207	O	PHE	229	15.385	26.202	75.014	1.00	22.15
	ATOM	208	N	LEU	230	17.487	25.899	74.263	1.00	20.44
	ATOM	209	CA	LEU	230	17.848	24.964	75.302	1.00	21.42
	ATOM	210	CB	LEU	230	18.255	23.631	74.650	1.00	20.34
5	ATOM	211	CG	LEU	230	17.191	22.855	73.834	1.00	22.70
	ATOM	212	CD1	LEU	230	17.860	21.762	73.013	1.00	23.14
	ATOM	213	CD2	LEU	230	16.130	22.252	74.773	1.00	21.55
	ATOM	214	C	LEU	230	19.017	25.540	76.094	1.00	20.71
	ATOM	215	O	LEU	230	19.977	26.038	75.524	1.00	20.61
10	ATOM	216	N	ARG	231	18.931	25.467	77.411	1.00	20.48
	ATOM	217	CA	ARG	231	20.018	25.997	78.211	1.00	20.62
	ATOM	218	CB	ARG	231	20.023	27.525	78.176	1.00	20.50
	ATOM	219	CG	ARG	231	18.907	28.184	79.017	1.00	24.52
	ATOM	220	CD	ARG	231	17.560	28.025	78.342	1.00	27.62
15	ATOM	221	NE	ARG	231	16.465	28.674	79.060	1.00	28.14
	ATOM	222	CZ	ARG	231	15.846	28.165	80.118	1.00	28.35
	ATOM	223	NH1	ARG	231	16.208	26.986	80.598	1.00	27.27
	ATOM	224	NH2	ARG	231	14.856	28.835	80.692	1.00	28.94
	ATOM	225	C	ARG	231	19.957	25.585	79.663	1.00	20.62
20	ATOM	226	O	ARG	231	18.884	25.350	80.219	1.00	20.08
	ATOM	227	N	VAL	232	21.138	25.549	80.265	1.00	20.70
	ATOM	228	CA	VAL	232	21.276	25.244	81.684	1.00	23.23
	ATOM	229	CB	VAL	232	22.596	24.499	81.961	1.00	24.57
	ATOM	230	CG1	VAL	232	22.800	24.335	83.460	1.00	24.88
25	ATOM	231	CG2	VAL	232	22.565	23.135	81.289	1.00	23.34
	ATOM	232	C	VAL	232	21.306	26.619	82.359	1.00	25.86
	ATOM	233	O	VAL	232	22.284	27.349	82.225	1.00	29.87
	ATOM	234	N	GLY	233	20.232	26.960	83.062	1.00	24.64
	ATOM	235	CA	GLY	233	20.137	28.249	83.730	1.00	26.40
30	ATOM	236	C	GLY	233	20.170	28.129	85.240	1.00	27.72
	ATOM	237	O	GLY	233	20.449	27.041	85.755	1.00	26.07
	ATOM	238	N	PRO	234	19.863	29.206	85.980	1.00	28.00
	ATOM	239	CD	PRO	234	19.340	30.507	85.515	1.00	30.45
	ATOM	240	CA	PRO	234	19.886	29.158	87.447	1.00	28.48
35	ATOM	241	CB	PRO	234	19.772	30.627	87.833	1.00	30.42
	ATOM	242	CG	PRO	234	18.804	31.123	86.802	1.00	32.04

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5	ATOM	243	C	PRO	234	18.752	28.323	88.037	1.00	27.91	
	ATOM	244	O	PRO	234	18.781	27.975	89.229	1.00	28.03	
	ATOM	245	N	ASP	235	17.757	27.996	87.210	1.00	26.13	
	ATOM	246	CA	ASP	235	16.636	27.186	87.680	1.00	23.93	
	ATOM	247	CB	ASP	235	15.333	27.686	87.064	1.00	28.77	
	ATOM	248	CG	ASP	235	15.405	27.820	85.544	1.00	31.24	
	ATOM	249	OD1	ASP	235	16.519	27.836	84.964	1.00	32.56	
	ATOM	250	OD2	ASP	235	14.327	27.922	84.919	1.00	34.70	
10	ATOM	251	C	ASP	235	16.828	25.700	87.362	1.00	20.99	
	ATOM	252	O	ASP	235	16.019	24.881	87.751	1.00	19.94	
	ATOM	253	N	SER	236	17.914	25.369	86.666	0.50	20.63	AC1
	ATOM	254	CA	SER	236	18.208	23.979	86.280	0.50	20.15	AC1
15	ATOM	255	CB	SER	236	19.196	23.969	85.111	0.50	19.44	AC1
	ATOM	256	OG	SER	236	18.708	24.734	84.013	0.50	19.16	AC1
	ATOM	257	C	SER	236	18.787	23.137	87.425	0.50	21.81	AC1
	ATOM	258	O	SER	236	19.849	23.457	87.946	0.50	20.58	AC1
20	ATOM	259	N	ASN	237	18.125	22.037	87.782	1.00	21.94	
	ATOM	260	CA	ASN	237	18.621	21.202	88.886	1.00	25.34	
	ATOM	261	CB	ASN	237	17.498	20.331	89.450	1.00	30.84	
	ATOM	262	CG	ASN	237	17.020	19.301	88.472	1.00	34.04	
	ATOM	263	OD1	ASN	237	17.786	18.838	87.623	1.00	39.37	
	ATOM	264	ND2	ASN	237	15.748	18.913	88.588	1.00	39.05	
	ATOM	265	C	ASN	237	19.843	20.325	88.581	1.00	26.93	
	ATOM	266	O	ASN	237	20.180	19.405	89.339	1.00	32.05	
25	ATOM	267	N	VAL	238	20.537	20.621	87.503	1.00	23.03	
	ATOM	268	CA	VAL	238	21.713	19.862	87.114	1.00	20.81	
	ATOM	269	CB	VAL	238	22.096	20.241	85.663	1.00	20.25	
	ATOM	270	CG1	VAL	238	23.336	19.495	85.207	1.00	19.20	
30	ATOM	271	CG2	VAL	238	20.919	19.922	84.741	1.00	20.14	
	ATOM	272	C	VAL	238	22.844	20.185	88.106	1.00	20.62	
	ATOM	273	O	VAL	238	23.147	21.343	88.363	1.00	18.94	
	ATOM	274	N	PRO	239	23.428	19.153	88.719	1.00	20.32	
35	ATOM	275	CD	PRO	239	23.144	17.726	88.541	1.00	20.40	
	ATOM	276	CA	PRO	239	24.515	19.328	89.688	1.00	21.49	
	ATOM	277	CB	PRO	239	24.911	17.892	90.023	1.00	22.13	
	ATOM	278	CG	PRO	239	23.696	17.174	89.847	1.00	20.51	

	ATOM	279	C	PRO	239	25.663	20.039	89.023	1.00	24.59
	ATOM	280	O	PRO	239	25.924	19.804	87.847	1.00	23.65
	ATOM	281	N	PRO	240	26.388	20.879	89.777	1.00	24.92
	ATOM	282	CD	PRO	240	26.142	21.311	91.167	1.00	26.02
5	ATOM	283	CA	PRO	240	27.524	21.603	89.202	1.00	26.88
	ATOM	284	CB	PRO	240	28.222	22.161	90.438	1.00	26.73
	ATOM	285	CG	PRO	240	27.039	22.543	91.299	1.00	29.18
	ATOM	286	C	PRO	240	28.434	20.733	88.363	1.00	26.35
	ATOM	287	O	PRO	240	28.847	21.125	87.259	1.00	27.72
10	ATOM	288	N	LYS	241	28.745	19.533	88.838	1.00	28.50
	ATOM	289	CA	LYS	241	29.642	18.682	88.071	1.00	28.19
	ATOM	290	CB	LYS	241	30.073	17.457	88.878	1.00	32.48
	ATOM	291	CG	LYS	241	28.970	16.508	89.292	1.00	34.64
	ATOM	292	CD	LYS	241	29.627	15.241	89.832	1.00	37.47
15	ATOM	293	CE	LYS	241	28.627	14.162	90.157	1.00	39.69
	ATOM	294	NZ	LYS	241	29.359	12.932	90.578	1.00	42.50
	ATOM	295	C	LYS	241	29.144	18.233	86.700	1.00	27.86
	ATOM	296	O	LYS	241	29.935	17.790	85.868	1.00	27.57
	ATOM	297	N	PHE	242	27.840	18.335	86.459	1.00	25.10
20	ATOM	298	CA	PHE	242	27.309	17.953	85.154	1.00	22.57
	ATOM	299	CB	PHE	242	26.161	16.954	85.319	1.00	24.91
	ATOM	300	CG	PHE	242	26.600	15.619	85.856	1.00	28.41
	ATOM	301	CD1	PHE	242	27.411	14.790	85.102	1.00	30.20
	ATOM	302	CD2	PHE	242	26.194	15.191	87.108	1.00	28.96
25	ATOM	303	CE1	PHE	242	27.813	13.544	85.583	1.00	31.58
	ATOM	304	CE2	PHE	242	26.594	13.943	87.596	1.00	30.20
	ATOM	305	CZ	PHE	242	27.400	13.127	86.832	1.00	32.03
	ATOM	306	C	PHE	242	26.837	19.151	84.330	1.00	19.63
	ATOM	307	O	PHE	242	26.386	18.991	83.190	1.00	20.79
30	ATOM	308	N	ARG	243	26.971	20.350	84.873	1.00	19.69
	ATOM	309	CA	ARG	243	26.513	21.529	84.153	1.00	20.41
	ATOM	310	CB	ARG	243	26.538	22.749	85.066	1.00	20.87
	ATOM	311	CG	ARG	243	25.523	22.602	86.208	1.00	23.08
	ATOM	312	CD	ARG	243	25.562	23.759	87.130	1.00	26.38
35	ATOM	313	NE	ARG	243	24.725	24.856	86.687	1.00	27.91
	ATOM	314	CZ	ARG	243	23.394	24.873	86.728	1.00	28.35

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	ATOM	315	NH1	ARG	243	22.697	23.825	87.192	1.00	26.91	
	ATOM	316	NH2	ARG	243	22.764	25.975	86.343	1.00	28.11	
	ATOM	317	C	ARG	243	27.238	21.813	82.846	1.00	20.13	
	ATOM	318	O	ARG	243	26.596	22.114	81.836	1.00	19.71	
5	ATOM	319	N	ALA	244	28.564	21.734	82.838	1.00	20.90	
	ATOM	320	CA	ALA	244	29.273	21.974	81.577	1.00	22.06	
	ATOM	321	CB	ALA	244	30.773	21.896	81.796	1.00	21.20	
	ATOM	322	C	ALA	244	28.842	20.984	80.492	1.00	21.05	
	ATOM	323	O	ALA	244	28.527	21.365	79.366	1.00	21.57	
10	ATOM	324	N	PRO	245	28.783	19.696	80.822	1.00	21.63	
	ATOM	325	CD	PRO	245	29.335	19.087	82.049	1.00	25.65	
	ATOM	326	CA	PRO	245	28.377	18.672	79.861	1.00	22.28	
	ATOM	327	CB	PRO	245	28.516	17.380	80.666	1.00	24.91	
	ATOM	328	CG	PRO	245	29.614	17.694	81.605	1.00	25.26	
15	ATOM	329	C	PRO	245	26.943	18.859	79.329	1.00	19.49	
	ATOM	330	O	PRO	245	26.691	18.778	78.118	1.00	21.31	
	ATOM	331	N	VAL	246	26.013	19.123	80.230	1.00	20.18	
	ATOM	332	CA	VAL	246	24.624	19.294	79.805	1.00	18.44	
	ATOM	333	CB	VAL	246	23.693	19.269	81.028	1.00	18.35	
20	ATOM	334	CG1	VAL	246	22.221	19.536	80.620	1.00	18.11	
	ATOM	335	CG2	VAL	246	23.766	17.845	81.678	1.00	17.69	
	ATOM	336	C	VAL	246	24.501	20.568	78.968	1.00	18.23	
	ATOM	337	O	VAL	246	23.773	20.603	77.977	1.00	18.23	
	ATOM	338	N	SER	247	25.234	21.609	79.351	0.50	20.08	AC1
25	ATOM	339	CA	SER	247	25.198	22.858	78.599	0.50	21.19	AC1
	ATOM	340	CB	SER	247	26.058	23.910	79.289	0.50	21.37	AC1
	ATOM	341	OG	SER	247	25.484	24.292	80.517	0.50	23.67	AC1
	ATOM	342	C	SER	247	25.712	22.621	77.189	0.50	21.32	AC1
	ATOM	343	O	SER	247	25.180	23.161	76.217	0.50	21.62	AC1
30	ATOM	344	N	SER	248	26.756	21.811	77.076	1.00	20.43	
	ATOM	345	CA	SER	248	27.322	21.502	75.766	1.00	21.62	
	ATOM	346	CB	SER	248	28.541	20.594	75.916	1.00	24.31	
	ATOM	347	OG	SER	248	29.660	21.350	76.354	1.00	24.89	
	ATOM	348	C	SER	248	26.271	20.800	74.903	1.00	22.36	
35	ATOM	349	O	SER	248	26.158	21.061	73.697	1.00	22.32	
	ATOM	350	N	LEU	249	25.513	19.895	75.519	1.00	22.35	

	ATOM	351	CA	LEU	249	24.462	19.185	74.791	1.00	22.28
	ATOM	352	CB	LEU	249	23.904	18.046	75.668	1.00	22.23
	ATOM	353	CG	LEU	249	24.970	16.972	75.954	1.00	25.52
	ATOM	354	CD1	LEU	249	24.441	15.919	76.922	1.00	26.39
5	ATOM	355	CD2	LEU	249	25.398	16.341	74.643	1.00	27.01
	ATOM	356	C	LEU	249	23.358	20.152	74.352	1.00	21.63
	ATOM	357	O	LEU	249	22.822	20.039	73.231	1.00	19.99
	ATOM	358	N	CYS	250	23.012	21.102	75.217	1.00	21.10
	ATOM	359	CA	CYS	250	21.995	22.098	74.856	1.00	21.22
10	ATOM	360	CB	CYS	250	21.701	23.044	76.019	1.00	20.65
	ATOM	361	SG	CYS	250	20.853	22.249	77.396	1.00	22.08
	ATOM	362	C	CYS	250	22.471	22.932	73.684	1.00	22.49
	ATOM	363	O	CYS	250	21.687	23.302	72.828	1.00	23.08
	ATOM	364	N	GLN	251	23.765	23.239	73.656	1.00	22.61
15	ATOM	365	CA	GLN	251	24.313	24.064	72.577	1.00	24.50
	ATOM	366	CB	GLN	251	25.738	24.482	72.925	1.00	26.13
	ATOM	367	CG	GLN	251	25.827	25.428	74.123	1.00	31.89
	ATOM	368	CD	GLN	251	27.270	25.602	74.609	1.00	36.32
	ATOM	369	OE1	GLN	251	28.146	26.020	73.846	1.00	38.70
20	ATOM	370	NE2	GLN	251	27.520	25.275	75.883	1.00	36.33
	ATOM	371	C	GLN	251	24.290	23.309	71.255	1.00	23.96
	ATOM	372	O	GLN	251	24.080	23.899	70.200	1.00	25.04
	ATOM	373	N	ILE	252	24.506	21.998	71.323	1.00	23.74
	ATOM	374	CA	ILE	252	24.475	21.143	70.140	1.00	24.05
25	ATOM	375	CB	ILE	252	24.877	19.690	70.493	1.00	25.71
	ATOM	376	CG2	ILE	252	24.385	18.727	69.419	1.00	25.12
	ATOM	377	CG1	ILE	252	26.405	19.596	70.658	1.00	26.17
	ATOM	378	CD1	ILE	252	26.874	18.335	71.359	1.00	27.45
	ATOM	379	C	ILE	252	23.032	21.183	69.642	1.00	25.30
30	ATOM	380	O	ILE	252	22.760	21.312	68.448	1.00	25.88
	ATOM	381	N	GLY	253	22.101	21.105	70.580	1.00	25.76
	ATOM	382	CA	GLY	253	20.698	21.167	70.213	1.00	24.72
	ATOM	383	C	GLY	253	20.327	22.497	69.573	1.00	24.98
	ATOM	384	O	GLY	253	19.611	22.527	68.561	1.00	24.56
35	ATOM	385	N	ASN	254	20.779	23.600	70.165	1.00	23.66
	ATOM	386	CA	ASN	254	20.483	24.929	69.642	1.00	24.18

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	ATOM	387	CB	ASN	254	21.063	25.999	70.566	1.00	23.04
	ATOM	388	CG	ASN	254	20.336	26.061	71.884	1.00	24.90
	ATOM	389	OD1	ASN	254	19.147	25.729	71.954	1.00	22.87
	ATOM	390	ND2	ASN	254	21.020	26.511	72.934	1.00	25.39
5	ATOM	391	C	ASN	254	20.990	25.142	68.215	1.00	25.59
	ATOM	392	O	ASN	254	20.349	25.832	67.418	1.00	25.49
	ATOM	393	N	LYS	255	22.154	24.575	67.915	1.00	24.87
	ATOM	394	CA	LYS	255	22.718	24.669	66.572	1.00	26.12
	ATOM	395	CB	LYS	255	24.121	24.061	66.518	1.00	29.40
10	ATOM	396	CG	LYS	255	25.162	24.983	67.112	1.00	33.68
	ATOM	397	CD	LYS	255	26.481	24.293	67.392	1.00	34.86
	ATOM	398	CE	LYS	255	27.280	24.027	66.150	1.00	35.57
	ATOM	399	NZ	LYS	255	28.719	23.853	66.527	1.00	33.75
	ATOM	400	C	LYS	255	21.816	23.924	65.608	1.00	26.04
15	ATOM	401	O	LYS	255	21.539	24.415	64.507	1.00	25.57
	ATOM	402	N	GLN	256	21.358	22.741	66.009	1.00	24.02
	ATOM	403	CA	GLN	256	20.498	21.967	65.121	1.00	23.89
	ATOM	404	CB	GLN	256	20.325	20.546	65.658	1.00	25.47
	ATOM	405	CG	GLN	256	21.676	19.880	65.887	1.00	28.63
20	ATOM	406	CD	GLN	256	21.565	18.517	66.534	1.00	30.93
	ATOM	407	OE1	GLN	256	20.710	18.301	67.387	1.00	32.63
	ATOM	408	NE2	GLN	256	22.439	17.599	66.149	1.00	30.18
	ATOM	409	C	GLN	256	19.156	22.658	64.915	1.00	24.45
	ATOM	410	O	GLN	256	18.596	22.598	63.828	1.00	24.20
25	ATOM	411	N	ILE	257	18.662	23.338	65.942	1.00	23.21
	ATOM	412	CA	ILE	257	17.390	24.059	65.816	1.00	22.41
	ATOM	413	CB	ILE	257	16.895	24.535	67.180	1.00	20.26
	ATOM	414	CG2	ILE	257	15.636	25.401	67.021	1.00	21.15
	ATOM	415	CG1	ILE	257	16.607	23.298	68.039	1.00	22.12
30	ATOM	416	CD1	ILE	257	16.309	23.620	69.517	1.00	21.36
	ATOM	417	C	ILE	257	17.558	25.253	64.877	1.00	23.91
	ATOM	418	O	ILE	257	16.677	25.544	64.060	1.00	21.49
	ATOM	419	N	ALA	258	18.684	25.949	64.994	1.00	23.86
	ATOM	420	CA	ALA	258	18.939	27.081	64.103	1.00	25.37
35	ATOM	421	CB	ALA	258	20.313	27.705	64.416	1.00	26.26
	ATOM	422	C	ALA	258	18.906	26.588	62.656	1.00	25.01

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	ATOM	423	O	ALA	258	18.306	27.238	61.783	1.00	25.91
	ATOM	424	N	ALA	259	19.555	25.450	62.403	1.00	23.72
	ATOM	425	CA	ALA	259	19.602	24.865	61.063	1.00	24.51
	ATOM	426	CB	ALA	259	20.442	23.613	61.058	1.00	24.62
5	ATOM	427	C	ALA	259	18.187	24.525	60.623	1.00	24.36
	ATOM	428	O	ALA	259	17.846	24.693	59.464	1.00	23.27
	ATOM	429	N	LEU	260	17.374	24.015	61.544	1.00	23.02
	ATOM	430	CA	LEU	260	15.986	23.685	61.188	1.00	24.75
	ATOM	431	CB	LEU	260	15.237	23.070	62.366	1.00	26.22
10	ATOM	432	CG	LEU	260	15.550	21.633	62.742	1.00	31.27
	ATOM	433	CD1	LEU	260	14.906	21.342	64.082	1.00	32.20
	ATOM	434	CD2	LEU	260	15.054	20.679	61.658	1.00	33.32
	ATOM	435	C	LEU	260	15.214	24.902	60.750	1.00	25.40
	ATOM	436	O	LEU	260	14.391	24.821	59.834	1.00	23.40
15	ATOM	437	N	VAL	261	15.439	26.031	61.419	1.00	25.21
	ATOM	438	CA	VAL	261	14.735	27.247	61.055	1.00	26.95
	ATOM	439	CB	VAL	261	15.050	28.411	62.036	1.00	25.46
	ATOM	440	CG1	VAL	261	14.386	29.700	61.544	1.00	27.40
	ATOM	441	CG2	VAL	261	14.520	28.075	63.434	1.00	27.42
20	ATOM	442	C	VAL	261	15.104	27.671	59.640	1.00	26.53
	ATOM	443	O	VAL	261	14.232	28.035	58.850	1.00	25.34
	ATOM	444	N	VAL	262	16.396	27.611	59.320	1.00	27.29
	ATOM	445	CA	VAL	262	16.874	27.995	57.993	1.00	28.11
	ATOM	446	CB	VAL	262	18.430	27.910	57.905	1.00	30.08
25	ATOM	447	CG1	VAL	262	18.883	27.872	56.441	1.00	33.75
	ATOM	448	CG2	VAL	262	19.051	29.104	58.606	1.00	32.97
	ATOM	449	C	VAL	262	16.267	27.075	56.939	1.00	26.73
	ATOM	450	O	VAL	262	15.909	27.511	55.840	1.00	26.28
	ATOM	451	N	TRP	263	16.177	25.794	57.286	1.00	24.38
30	ATOM	452	CA	TRP	263	15.623	24.775	56.402	1.00	25.26
	ATOM	453	CB	TRP	263	15.831	23.406	57.052	1.00	23.10
	ATOM	454	CG	TRP	263	15.102	22.286	56.409	1.00	24.27
	ATOM	455	CD2	TRP	263	13.881	21.697	56.873	1.00	24.86
	ATOM	456	CE2	TRP	263	13.536	20.681	55.962	1.00	25.93
35	ATOM	457	CE3	TRP	263	13.051	21.936	57.974	1.00	24.53
	ATOM	458	CD1	TRP	263	15.441	21.624	55.267	1.00	24.80

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	ATOM	459	NE1 TRP	263	14.501	20.655	54.990	1.00	27.16
	ATOM	460	CZ2 TRP	263	12.391	19.895	56.115	1.00	26.26
	ATOM	461	CZ3 TRP	263	11.911	21.151	58.132	1.00	23.32
	ATOM	462	CH2 TRP	263	11.598	20.144	57.204	1.00	23.73
5	ATOM	463	C TRP	263	14.125	25.047	56.175	1.00	24.66
	ATOM	464	O TRP	263	13.645	25.081	55.037	1.00	25.81
	ATOM	465	N ALA	264	13.391	25.278	57.252	1.00	24.56
	ATOM	466	CA ALA	264	11.949	25.506	57.103	1.00	25.04
	ATOM	467	CB ALA	264	11.304	25.733	58.464	1.00	26.00
10	ATOM	468	C ALA	264	11.675	26.701	56.205	1.00	27.22
	ATOM	469	O ALA	264	10.838	26.640	55.293	1.00	24.71
	ATOM	470	N ARG	265	12.372	27.794	56.489	1.00	28.16
	ATOM	471	CA ARG	265	12.227	29.024	55.724	1.00	32.11
	ATOM	472	CB ARG	265	13.250	30.066	56.218	1.00	33.47
15	ATOM	473	CG ARG	265	13.155	31.408	55.520	1.00	36.25
	ATOM	474	CD ARG	265	14.169	32.397	56.078	1.00	39.06
	ATOM	475	NE ARG	265	15.545	31.972	55.823	1.00	42.06
	ATOM	476	CZ ARG	265	16.609	32.534	56.391	1.00	43.94
	ATOM	477	NH1 ARG	265	16.447	33.541	57.244	1.00	44.49
20	ATOM	478	NH2 ARG	265	17.827	32.092	56.110	1.00	43.52
	ATOM	479	C ARG	265	12.424	28.767	54.225	1.00	32.76
	ATOM	480	O ARG	265	11.843	29.460	53.392	1.00	35.61
	ATOM	481	N ASP	266	13.227	27.771	53.872	1.00	33.71
	ATOM	482	CA ASP	266	13.465	27.492	52.466	1.00	34.17
25	ATOM	483	CB ASP	266	14.931	27.106	52.236	1.00	37.32
	ATOM	484	CG ASP	266	15.879	28.293	52.374	1.00	40.62
	ATOM	485	OD1 ASP	266	15.556	29.392	51.866	1.00	40.66
	ATOM	486	OD2 ASP	266	16.959	28.128	52.985	1.00	43.94
	ATOM	487	C ASP	266	12.544	26.447	51.833	1.00	33.93
30	ATOM	488	O ASP	266	12.664	26.156	50.646	1.00	32.38
	ATOM	489	N ILE	267	11.640	25.869	52.619	1.00	32.18
	ATOM	490	CA ILE	267	10.694	24.897	52.077	1.00	30.21
	ATOM	491	CB ILE	267	9.820	24.279	53.210	1.00	29.16
	ATOM	492	CG2 ILE	267	8.586	23.588	52.620	1.00	31.21
35	ATOM	493	CG1 ILE	267	10.643	23.291	54.038	1.00	29.01
	ATOM	494	CD1 ILE	267	11.069	22.051	53.278	1.00	28.89

	ATOM	495	C	ILE	267	9.800	25.670	51.093	1.00	30.06	
	ATOM	496	O	ILE	267	9.256	26.715	51.421	1.00	29.41	
	ATOM	497	N	PRO	268	9.653	25.164	49.862	1.00	31.41	
	ATOM	498	CD	PRO	268	10.216	23.921	49.300	1.00	31.06	
5	ATOM	499	CA	PRO	268	8.813	25.857	48.879	1.00	31.62	
	ATOM	500	CB	PRO	268	8.686	24.830	47.755	1.00	31.63	
	ATOM	501	CG	PRO	268	10.012	24.126	47.811	1.00	34.16	
	ATOM	502	C	PRO	268	7.459	26.286	49.444	1.00	31.83	
	ATOM	503	O	PRO	268	6.762	25.483	50.051	1.00	31.61	
10	ATOM	504	N	HIS	269	7.128	27.566	49.267	1.00	31.08	
	ATOM	505	CA	HIS	269	5.867	28.164	49.715	1.00	31.47	
	ATOM	506	CB	HIS	269	4.677	27.277	49.300	1.00	33.82	
	ATOM	507	CG	HIS	269	4.710	26.845	47.865	1.00	36.44	
	ATOM	508	CD2	HIS	269	4.694	25.611	47.305	1.00	37.13	
15	ATOM	509	ND1	HIS	269	4.734	27.740	46.816	1.00	39.48	
	ATOM	510	CE1	HIS	269	4.731	27.078	45.672	1.00	37.91	
	ATOM	511	NE2	HIS	269	4.706	25.785	45.941	1.00	39.31	
	ATOM	512	C	HIS	269	5.745	28.465	51.210	1.00	30.01	
	ATOM	513	O	HIS	269	4.796	29.133	51.638	1.00	28.74	
20	ATOM	514	N	PHE	270	6.693	27.994	52.012	1.00	28.26	
	ATOM	515	CA	PHE	270	6.607	28.222	53.454	1.00	27.87	
	ATOM	516	CB	PHE	270	7.728	27.468	54.178	1.00	26.66	
	ATOM	517	CG	PHE	270	7.661	27.563	55.684	1.00	24.18	
	ATOM	518	CD1	PHE	270	6.867	26.683	56.415	1.00	24.15	
25	ATOM	519	CD2	PHE	270	8.385	28.536	56.372	1.00	26.34	
	ATOM	520	CE1	PHE	270	6.792	26.775	57.822	1.00	22.45	
	ATOM	521	CE2	PHE	270	8.316	28.637	57.778	1.00	24.45	
	ATOM	522	CZ	PHE	270	7.516	27.754	58.494	1.00	23.03	
	ATOM	523	C	PHE	270	6.650	29.707	53.811	1.00	28.65	
30	ATOM	524	O	PHE	270	5.866	30.175	54.634	1.00	29.19	
	ATOM	525	N	SER	271	7.558	30.448	53.184	0.50	29.83	AC1
	ATOM	526	CA	SER	271	7.676	31.876	53.463	0.50	31.34	AC1
	ATOM	527	CB	SER	271	8.959	32.432	52.839	0.50	31.74	AC1
	ATOM	528	OG	SER	271	10.104	31.869	53.460	0.50	31.64	AC1
35	ATOM	529	C	SER	271	6.458	32.663	52.974	0.50	32.85	AC1
	ATOM	530	O	SER	271	6.301	33.839	53.296	0.50	33.99	AC1

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	ATOM	531	N	GLN	272	5.599	32.009	52.197	1.00	33.79
	ATOM	532	CA	GLN	272	4.378	32.642	51.696	1.00	35.22
	ATOM	533	CB	GLN	272	3.910	31.928	50.423	1.00	39.02
	ATOM	534	CG	GLN	272	4.777	32.210	49.191	1.00	43.59
5	ATOM	535	CD	GLN	272	4.608	31.169	48.086	1.00	45.89
	ATOM	536	OE1	GLN	272	3.488	30.794	47.727	1.00	47.68
	ATOM	537	NE2	GLN	272	5.729	30.703	47.534	1.00	48.15
	ATOM	538	C	GLN	272	3.255	32.633	52.742	1.00	35.20
	ATOM	539	O	GLN	272	2.288	33.397	52.648	1.00	33.55
10	ATOM	540	N	LEU	273	3.383	31.756	53.736	1.00	33.18
	ATOM	541	CA	LEU	273	2.402	31.651	54.811	1.00	31.26
	ATOM	542	CB	LEU	273	2.695	30.398	55.653	1.00	30.14
	ATOM	543	CG	LEU	273	2.671	29.015	54.988	1.00	29.04
	ATOM	544	CD1	LEU	273	3.273	27.989	55.930	1.00	28.99
15	ATOM	545	CD2	LEU	273	1.231	28.638	54.645	1.00	29.21
	ATOM	546	C	LEU	273	2.500	32.880	55.722	1.00	30.95
	ATOM	547	O	LEU	273	3.556	33.513	55.793	1.00	30.58
	ATOM	548	N	GLU	274	1.416	33.208	56.420	1.00	31.28
	ATOM	549	CA	GLU	274	1.435	34.332	57.355	1.00	32.85
20	ATOM	550	CB	GLU	274	0.154	34.378	58.195	1.00	35.60
	ATOM	551	CG	GLU	274	-1.039	35.022	57.511	1.00	40.50
	ATOM	552	CD	GLU	274	-0.954	36.543	57.494	1.00	43.35
	ATOM	553	OE1	GLU	274	-1.788	37.171	56.807	1.00	44.88
	ATOM	554	OE2	GLU	274	-0.062	37.109	58.169	1.00	45.29
25	ATOM	555	C	GLU	274	2.615	34.079	58.287	1.00	32.91
	ATOM	556	O	GLU	274	2.867	32.936	58.693	1.00	31.56
	ATOM	557	N	MET	275	3.331	35.136	58.632	1.00	31.54
	ATOM	558	CA	MET	275	4.483	35.010	59.507	1.00	31.78
	ATOM	559	CB	MET	275	5.094	36.392	59.748	1.00	34.73
30	ATOM	560	CG	MET	275	6.288	36.403	60.673	1.00	37.61
	ATOM	561	SD	MET	275	7.574	35.262	60.158	1.00	39.49
	ATOM	562	CE	MET	275	7.940	35.869	58.496	1.00	39.54
	ATOM	563	C	MET	275	4.149	34.351	60.838	1.00	31.91
	ATOM	564	O	MET	275	4.885	33.474	61.305	1.00	31.90
35	ATOM	565	N	GLU	276	3.052	34.764	61.458	1.00	31.07
	ATOM	566	CA	GLU	276	2.684	34.184	62.736	1.00	30.79

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	ATOM	567	CB	GLU	276	1.499	34.938	63.341	1.00	35.06
	ATOM	568	CG	GLU	276	1.866	36.382	63.755	1.00	37.66
	ATOM	569	CD	GLU	276	3.043	36.434	64.731	1.00	40.34
	ATOM	570	OE1	GLU	276	2.978	35.751	65.774	1.00	41.45
5	ATOM	571	OE2	GLU	276	4.034	37.157	64.464	1.00	42.59
	ATOM	572	C	GLU	276	2.388	32.693	62.596	1.00	29.05
	ATOM	573	O	GLU	276	2.529	31.946	63.559	1.00	28.93
	ATOM	574	N	ASP	277	1.973	32.250	61.411	1.00	26.93
	ATOM	575	CA	ASP	277	1.716	30.817	61.223	1.00	24.95
10	ATOM	576	CB	ASP	277	0.817	30.565	60.005	1.00	26.30
	ATOM	577	CG	ASP	277	-0.656	30.768	60.320	1.00	26.04
	ATOM	578	OD1	ASP	277	-0.984	31.102	61.476	1.00	29.19
	ATOM	579	OD2	ASP	277	-1.492	30.596	59.410	1.00	26.42
	ATOM	580	C	ASP	277	3.056	30.089	61.069	1.00	25.34
15	ATOM	581	O	ASP	277	3.226	28.967	61.579	1.00	25.43
	ATOM	582	N	GLN	278	4.007	30.721	60.373	1.00	23.47
	ATOM	583	CA	GLN	278	5.338	30.132	60.203	1.00	23.93
	ATOM	584	CB	GLN	278	6.275	31.094	59.467	1.00	23.08
	ATOM	585	CG	GLN	278	5.931	31.265	57.999	1.00	26.36
20	ATOM	586	CD	GLN	278	6.858	32.238	57.324	1.00	26.00
	ATOM	587	OE1	GLN	278	8.075	32.122	57.439	1.00	26.10
	ATOM	588	NE2	GLN	278	6.293	33.210	56.609	1.00	28.94
	ATOM	589	C	GLN	278	5.917	29.850	61.588	1.00	22.78
	ATOM	590	O	GLN	278	6.445	28.765	61.857	1.00	20.87
25	ATOM	591	N	ILE	279	5.821	30.849	62.461	1.00	23.32
	ATOM	592	CA	ILE	279	6.322	30.719	63.825	1.00	22.80
	ATOM	593	CB	ILE	279	6.125	32.046	64.591	1.00	24.62
	ATOM	594	CG2	ILE	279	6.449	31.868	66.076	1.00	24.08
	ATOM	595	CG1	ILE	279	6.997	33.125	63.943	1.00	27.52
30	ATOM	596	CD1	ILE	279	6.728	34.543	64.464	1.00	27.69
	ATOM	597	C	ILE	279	5.638	29.560	64.573	1.00	22.81
	ATOM	598	O	ILE	279	6.294	28.758	65.215	1.00	23.50
	ATOM	599	N	LEU	280	4.318	29.463	64.498	1.00	20.16
	ATOM	600	CA	LEU	280	3.653	28.382	65.186	1.00	18.30
35	ATOM	601	CB	LEU	280	2.125	28.553	65.113	1.00	19.64
	ATOM	602	CG	LEU	280	1.589	29.739	65.931	1.00	22.60

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	ATOM	603	CD1	LEU	280	0.093	29.931	65.623	1.00	24.59
	ATOM	604	CD2	LEU	280	1.759	29.496	67.399	1.00	25.05
	ATOM	605	C	LEU	280	4.045	27.028	64.653	1.00	17.14
	ATOM	606	O	LEU	280	4.160	26.084	65.436	1.00	18.84
5	ATOM	607	N	LEU	281	4.225	26.905	63.335	1.00	17.52
	ATOM	608	CA	LEU	281	4.586	25.591	62.773	1.00	19.05
	ATOM	609	CB	LEU	281	4.550	25.618	61.241	1.00	19.60
	ATOM	610	CG	LEU	281	3.167	25.782	60.595	1.00	21.40
	ATOM	611	CD1	LEU	281	3.324	25.870	59.073	1.00	23.62
10	ATOM	612	CD2	LEU	281	2.266	24.621	60.975	1.00	21.20
	ATOM	613	C	LEU	281	5.968	25.143	63.255	1.00	19.84
	ATOM	614	O	LEU	281	6.164	23.977	63.620	1.00	19.38
	ATOM	615	N	ILE	282	6.923	26.067	63.269	1.00	20.43
	ATOM	616	CA	ILE	282	8.270	25.740	63.731	1.00	19.64
15	ATOM	617	CB	ILE	282	9.274	26.881	63.361	1.00	20.44
	ATOM	618	CG2	ILE	282	10.619	26.706	64.102	1.00	20.04
	ATOM	619	CG1	ILE	282	9.486	26.873	61.839	1.00	20.45
	ATOM	620	CD1	ILE	282	10.278	28.076	61.323	1.00	22.03
	ATOM	621	C	ILE	282	8.255	25.496	65.239	1.00	19.41
20	ATOM	622	O	ILE	282	8.894	24.574	65.717	1.00	19.21
	ATOM	623	N	LYS	283	7.533	26.322	65.992	1.00	17.59
	ATOM	624	CA	LYS	283	7.480	26.148	67.446	1.00	19.01
	ATOM	625	CB	LYS	283	6.624	27.246	68.103	1.00	19.89
	ATOM	626	CG	LYS	283	6.596	27.154	69.613	1.00	23.82
25	ATOM	627	CD	LYS	283	5.948	28.388	70.243	1.00	26.99
	ATOM	628	CE	LYS	283	5.645	28.183	71.731	1.00	30.98
	ATOM	629	NZ	LYS	283	6.837	27.917	72.599	1.00	34.38
	ATOM	630	C	LYS	283	6.873	24.791	67.778	1.00	19.44
	ATOM	631	O	LYS	283	7.274	24.120	68.729	1.00	19.31
30	ATOM	632	N	GLY	284	5.882	24.390	66.983	1.00	19.18
	ATOM	633	CA	GLY	284	5.240	23.124	67.254	1.00	18.56
	ATOM	634	C	GLY	284	5.981	21.885	66.806	1.00	18.31
	ATOM	635	O	GLY	284	5.731	20.805	67.328	1.00	19.56
	ATOM	636	N	SER	285	6.941	22.024	65.895	1.00	18.65
35	ATOM	637	CA	SER	285	7.633	20.844	65.384	1.00	17.51
	ATOM	638	CB	SER	285	7.453	20.755	63.870	1.00	19.70

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	ATOM	639	OG	SER	285	8.063	21.874	63.212	1.00	18.48
	ATOM	640	C	SER	285	9.136	20.728	65.663	1.00	15.25
	ATOM	641	O	SER	285	9.705	19.673	65.406	1.00	15.43
	ATOM	642	N	TRP	286	9.770	21.759	66.203	1.00	15.99
5	ATOM	643	CA	TRP	286	11.221	21.642	66.395	1.00	16.28
	ATOM	644	CB	TRP	286	11.812	22.920	67.007	1.00	17.10
	ATOM	645	CG	TRP	286	11.458	23.226	68.414	1.00	17.32
	ATOM	646	CD2	TRP	286	12.117	22.736	69.592	1.00	18.06
	ATOM	647	CE2	TRP	286	11.440	23.291	70.709	1.00	20.12
10	ATOM	648	CE3	TRP	286	13.208	21.882	69.815	1.00	17.92
	ATOM	649	CD1	TRP	286	10.445	24.033	68.850	1.00	18.61
	ATOM	650	NE1	TRP	286	10.427	24.076	70.227	1.00	18.32
	ATOM	651	CZ2	TRP	286	11.816	23.020	72.027	1.00	17.23
	ATOM	652	CZ3	TRP	286	13.580	21.608	71.136	1.00	18.42
15	ATOM	653	CH2	TRP	286	12.889	22.172	72.219	1.00	19.75
	ATOM	654	C	TRP	286	11.668	20.443	67.219	1.00	16.59
	ATOM	655	O	TRP	286	12.655	19.766	66.886	1.00	17.31
	ATOM	656	N	ASN	287	10.938	20.167	68.282	1.00	15.26
	ATOM	657	CA	ASN	287	11.301	19.059	69.157	1.00	14.41
20	ATOM	658	CB	ASN	287	10.508	19.180	70.456	1.00	17.68
	ATOM	659	CG	ASN	287	10.894	18.145	71.474	1.00	19.61
	ATOM	660	OD1	ASN	287	11.757	18.374	72.348	1.00	23.92
	ATOM	661	ND2	ASN	287	10.251	16.991	71.384	1.00	18.83
	ATOM	662	C	ASN	287	11.096	17.718	68.448	1.00	14.74
25	ATOM	663	O	ASN	287	11.954	16.846	68.508	1.00	16.16
	ATOM	664	N	GLU	288	9.966	17.555	67.752	1.00	15.22
	ATOM	665	CA	GLU	288	9.745	16.319	66.986	1.00	16.77
	ATOM	666	CB	GLU	288	8.367	16.358	66.288	1.00	17.55
	ATOM	667	CG	GLU	288	7.213	16.044	67.224	1.00	18.68
30	ATOM	668	CD	GLU	288	5.868	16.134	66.548	1.00	23.02
	ATOM	669	OE1	GLU	288	5.786	15.849	65.342	1.00	28.18
	ATOM	670	OE2	GLU	288	4.887	16.461	67.243	1.00	29.07
	ATOM	671	C	GLU	288	10.838	16.122	65.921	1.00	17.49
	ATOM	672	O	GLU	288	11.338	15.014	65.743	1.00	16.93
35	ATOM	673	N	LEU	289	11.193	17.204	65.220	1.00	14.56
	ATOM	674	CA	LEU	289	12.196	17.130	64.173	1.00	15.76

	ATOM	675	CB	LEU	289	12.248	18.451	63.390	1.00	14.77
	ATOM	676	CG	LEU	289	11.006	18.639	62.483	1.00	16.67
	ATOM	677	CD1	LEU	289	10.932	20.093	62.002	1.00	18.25
	ATOM	678	CD2	LEU	289	11.083	17.667	61.287	1.00	15.71
5	ATOM	679	C	LEU	289	13.555	16.784	64.752	1.00	16.05
	ATOM	680	O	LEU	289	14.301	16.022	64.138	1.00	16.56
	ATOM	681	N	LEU	290	13.884	17.312	65.929	1.00	16.37
	ATOM	682	CA	LEU	290	15.190	16.951	66.529	1.00	16.68
	ATOM	683	CB	LEU	290	15.477	17.734	67.809	1.00	17.02
10	ATOM	684	CG	LEU	290	15.786	19.219	67.684	1.00	22.29
	ATOM	685	CD1	LEU	290	16.294	19.726	69.046	1.00	23.74
	ATOM	686	CD2	LEU	290	16.865	19.454	66.604	1.00	25.08
	ATOM	687	C	LEU	290	15.229	15.471	66.868	1.00	16.18
	ATOM	688	O	LEU	290	16.214	14.803	66.605	1.00	17.45
15	ATOM	689	N	LEU	291	14.142	14.958	67.465	1.00	16.16
	ATOM	690	CA	LEU	291	14.088	13.553	67.826	1.00	17.64
	ATOM	691	CB	LEU	291	12.828	13.289	68.666	1.00	17.32
	ATOM	692	CG	LEU	291	12.824	13.961	70.046	1.00	20.40
	ATOM	693	CD1	LEU	291	11.405	13.964	70.627	1.00	22.18
20	ATOM	694	CD2	LEU	291	13.789	13.222	70.971	1.00	23.46
	ATOM	695	C	LEU	291	14.087	12.662	66.595	1.00	15.65
	ATOM	696	O	LEU	291	14.645	11.569	66.611	1.00	17.39
	ATOM	697	N	PHE	292	13.434	13.116	65.520	1.00	14.81
	ATOM	698	CA	PHE	292	13.360	12.330	64.311	1.00	15.62
25	ATOM	699	CB	PHE	292	12.392	12.993	63.314	1.00	16.43
	ATOM	700	CG	PHE	292	12.003	12.113	62.167	1.00	16.59
	ATOM	701	CD1	PHE	292	11.588	10.812	62.389	1.00	18.96
	ATOM	702	CD2	PHE	292	12.002	12.607	60.875	1.00	19.01
	ATOM	703	CE1	PHE	292	11.170	10.011	61.332	1.00	20.62
30	ATOM	704	CE2	PHE	292	11.581	11.805	59.805	1.00	18.46
	ATOM	705	CZ	PHE	292	11.166	10.499	60.060	1.00	18.06
	ATOM	706	C	PHE	292	14.761	12.191	63.713	1.00	15.70
	ATOM	707	O	PHE	292	15.132	11.119	63.236	1.00	15.72
	ATOM	708	N	ALA	293	15.526	13.278	63.760	1.00	16.34
35	ATOM	709	CA	ALA	293	16.906	13.267	63.232	1.00	16.73
	ATOM	710	CB	ALA	293	17.464	14.702	63.207	1.00	17.74

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	ATOM	711	C	ALA	293	17.802	12.368	64.090	1.00	17.09
	ATOM	712	O	ALA	293	18.668	11.654	63.570	1.00	17.27
	ATOM	713	N	ILE	294	17.623	12.423	65.407	1.00	16.09
	ATOM	714	CA	ILE	294	18.389	11.569	66.312	1.00	16.22
5	ATOM	715	CB	ILE	294	18.032	11.857	67.768	1.00	15.67
	ATOM	716	CG2	ILE	294	18.584	10.765	68.679	1.00	16.66
	ATOM	717	CG1	ILE	294	18.615	13.218	68.160	1.00	17.00
	ATOM	718	CD1	ILE	294	18.206	13.635	69.535	1.00	20.77
	ATOM	719	C	ILE	294	18.070	10.111	65.971	1.00	16.74
10	ATOM	720	O	ILE	294	18.954	9.296	65.833	1.00	16.38
	ATOM	721	N	ALA	295	16.791	9.791	65.774	1.00	16.15
	ATOM	722	CA	ALA	295	16.452	8.420	65.424	1.00	16.99
	ATOM	723	CB	ALA	295	14.937	8.273	65.332	1.00	16.54
	ATOM	724	C	ALA	295	17.083	7.993	64.088	1.00	17.97
15	ATOM	725	O	ALA	295	17.563	6.870	63.954	1.00	18.01
	ATOM	726	N	TRP	296	17.071	8.881	63.102	1.00	18.59
	ATOM	727	CA	TRP	296	17.625	8.570	61.782	1.00	18.81
	ATOM	728	CB	TRP	296	17.321	9.740	60.835	1.00	20.21
	ATOM	729	CG	TRP	296	17.849	9.622	59.451	1.00	22.61
20	ATOM	730	CD2	TRP	296	17.398	8.716	58.433	1.00	25.62
	ATOM	731	CE2	TRP	296	18.125	9.007	57.265	1.00	26.25
	ATOM	732	CE3	TRP	296	16.448	7.683	58.402	1.00	25.95
	ATOM	733	CD1	TRP	296	18.807	10.403	58.871	1.00	26.23
	ATOM	734	NE1	TRP	296	18.975	10.043	57.556	1.00	26.50
25	ATOM	735	CZ2	TRP	296	17.934	8.297	56.063	1.00	27.77
	ATOM	736	CZ3	TRP	296	16.257	6.977	57.206	1.00	27.65
	ATOM	737	CH2	TRP	296	16.996	7.289	56.061	1.00	25.35
	ATOM	738	C	TRP	296	19.133	8.299	61.878	1.00	19.53
	ATOM	739	O	TRP	296	19.647	7.296	61.345	1.00	21.43
30	ATOM	740	N	ARG	297	19.833	9.147	62.623	1.00	18.58
	ATOM	741	CA	ARG	297	21.280	8.974	62.748	1.00	18.22
	ATOM	742	CB	ARG	297	21.923	10.208	63.376	1.00	18.92
	ATOM	743	CG	ARG	297	21.886	11.465	62.525	1.00	20.63
	ATOM	744	CD	ARG	297	22.792	12.530	63.137	1.00	26.15
35	ATOM	745	NE	ARG	297	22.219	13.002	64.381	1.00	29.32
	ATOM	746	CZ	ARG	297	21.393	14.040	64.462	1.00	28.97

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	ATOM	747	NH1	ARG	297	21.066	14.720	63.373	1.00	29.81
	ATOM	748	NH2	ARG	297	20.872	14.372	65.628	1.00	31.03
	ATOM	749	C	ARG	297	21.643	7.776	63.605	1.00	18.87
	ATOM	750	O	ARG	297	22.738	7.225	63.473	1.00	19.01
5	ATOM	751	N	SER	298	20.749	7.404	64.511	1.00	17.52
	ATOM	752	CA	SER	298	21.023	6.293	65.414	1.00	18.09
	ATOM	753	CB	SER	298	20.134	6.407	66.655	1.00	18.94
	ATOM	754	OG	SER	298	20.412	7.606	67.381	1.00	18.16
	ATOM	755	C	SER	298	20.865	4.929	64.770	1.00	20.63
10	ATOM	756	O	SER	298	21.310	3.925	65.336	1.00	24.22
	ATOM	757	N	MET	299	20.270	4.868	63.582	1.00	20.01
	ATOM	758	CA	MET	299	20.106	3.558	62.953	1.00	22.16
	ATOM	759	CB	MET	299	19.367	3.682	61.610	1.00	24.42
	ATOM	760	CG	MET	299	17.940	4.159	61.735	1.00	24.29
15	ATOM	761	SD	MET	299	17.091	4.052	60.130	1.00	31.30
	ATOM	762	CE	MET	299	18.221	4.950	59.082	1.00	31.06
	ATOM	763	C	MET	299	21.431	2.825	62.725	1.00	25.30
	ATOM	764	O	MET	299	21.493	1.600	62.859	1.00	26.84
	ATOM	765	N	GLU	300	22.485	3.565	62.414	1.00	28.43
20	ATOM	766	CA	GLU	300	23.775	2.944	62.117	1.00	32.11
	ATOM	767	CB	GLU	300	24.736	3.949	61.472	1.00	34.60
	ATOM	768	CG	GLU	300	25.355	4.941	62.420	1.00	40.06
	ATOM	769	CD	GLU	300	26.689	5.477	61.910	1.00	43.56
	ATOM	770	OE1	GLU	300	27.622	4.666	61.729	1.00	46.83
25	ATOM	771	OE2	GLU	300	26.812	6.703	61.688	1.00	45.34
	ATOM	772	C	GLU	300	24.467	2.304	63.300	1.00	32.94
	ATOM	773	O	GLU	300	25.389	1.517	63.123	1.00	32.67
	ATOM	774	N	PHE	301	24.033	2.649	64.507	1.00	31.51
	ATOM	775	CA	PHE	301	24.632	2.094	65.710	1.00	32.60
30	ATOM	776	CB	PHE	301	24.822	3.214	66.736	1.00	32.49
	ATOM	777	CG	PHE	301	25.879	4.203	66.349	1.00	34.07
	ATOM	778	CD1	PHE	301	27.223	3.838	66.358	1.00	33.32
	ATOM	779	CD2	PHE	301	25.537	5.483	65.929	1.00	33.10
	ATOM	780	CE1	PHE	301	28.207	4.737	65.949	1.00	34.17
35	ATOM	781	CE2	PHE	301	26.506	6.385	65.519	1.00	34.69
	ATOM	782	CZ	PHE	301	27.854	6.008	65.530	1.00	33.21

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	ATOM	783	C	PHE	301	23.820	0.940	66.301	1.00	33.77
	ATOM	784	O	PHE	301	24.127	0.441	67.377	1.00	34.55
	ATOM	785	N	LEU	302	22.780	0.516	65.589	1.00	34.80
	ATOM	786	CA	LEU	302	21.966	-0.593	66.045	1.00	36.81
5	ATOM	787	CB	LEU	302	20.641	-0.645	65.287	1.00	34.98
	ATOM	788	CG	LEU	302	19.779	0.596	65.488	1.00	31.61
	ATOM	789	CD1	LEU	302	18.551	0.528	64.577	1.00	31.62
	ATOM	790	CD2	LEU	302	19.386	0.717	66.955	1.00	31.48
	ATOM	791	C	LEU	302	22.744	-1.869	65.775	1.00	40.52
10	ATOM	792	O	LEU	302	23.333	-2.038	64.701	1.00	40.16
	ATOM	793	N	THR	303	22.733	-2.764	66.753	1.00	44.10
	ATOM	794	CA	THR	303	23.422	-4.037	66.634	1.00	48.80
	ATOM	795	CB	THR	303	23.126	-4.933	67.850	1.00	49.83
	ATOM	796	OG1	THR	303	23.211	-4.151	69.050	1.00	51.18
15	ATOM	797	CG2	THR	303	24.132	-6.076	67.924	1.00	51.25
	ATOM	798	C	THR	303	22.932	-4.731	65.368	1.00	50.84
	ATOM	799	O	THR	303	21.739	-4.703	65.052	1.00	50.20
	ATOM	800	N	ALA	304	23.864	-5.341	64.644	1.00	53.24
	ATOM	801	CA	ALA	304	23.538	-6.040	63.410	1.00	55.88
20	ATOM	802	CB	ALA	304	24.739	-6.867	62.946	1.00	56.05
	ATOM	803	C	ALA	304	22.317	-6.942	63.575	1.00	57.61
	ATOM	804	O	ALA	304	22.133	-7.583	64.617	1.00	58.45
	ATOM	805	N	ALA	305	21.481	-6.972	62.540	1.00	59.51
	ATOM	806	CA	ALA	305	20.282	-7.797	62.535	1.00	60.68
25	ATOM	807	CB	ALA	305	19.548	-7.651	61.205	1.00	60.98
	ATOM	808	C	ALA	305	20.714	-9.245	62.744	1.00	61.71
	ATOM	809	O	ALA	305	19.925	-10.029	63.319	1.00	62.15
	ATOM	810	OXT	ALA	305	21.848	-9.572	62.316	1.00	61.88
	ATOM	811	CB	ALA	316	17.484	-11.402	70.435	1.00	59.02
30	ATOM	812	C	ALA	316	15.833	-9.781	71.403	1.00	57.95
	ATOM	813	O	ALA	316	15.469	-9.327	70.316	1.00	58.69
	ATOM	814	N	ALA	316	15.341	-12.224	71.375	1.00	58.18
	ATOM	815	CA	ALA	316	16.413	-11.191	71.510	1.00	58.61
	ATOM	816	N	ALA	317	15.747	-9.096	72.539	1.00	56.79
35	ATOM	817	CA	ALA	317	15.218	-7.739	72.587	1.00	54.70
	ATOM	818	CB	ALA	317	13.813	-7.745	73.174	1.00	54.73

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	ATOM	819	C	ALA	317	16.142	-6.871	73.437	1.00	52.91	
	ATOM	820	O	ALA	317	15.697	-5.935	74.111	1.00	53.06	
	ATOM	821	N	SER	318	17.430	-7.207	73.404	1.00	49.42	
	ATOM	822	CA	SER	318	18.449	-6.478	74.151	1.00	46.14	
5	ATOM	823	CB	SER	318	19.830	-7.056	73.835	1.00	46.72	
	ATOM	824	OG	SER	318	20.834	-6.462	74.639	1.00	47.98	
	ATOM	825	C	SER	318	18.378	-5.009	73.723	1.00	43.02	
	ATOM	826	O	SER	318	18.543	-4.686	72.541	1.00	44.27	
	ATOM	827	N	PRO	319	18.122	-4.100	74.676	0.50	41.03	AC1
10	ATOM	828	CD	PRO	319	17.740	-4.342	76.079	0.50	40.29	AC1
	ATOM	829	CA	PRO	319	18.033	-2.672	74.351	0.50	38.31	AC1
	ATOM	830	CB	PRO	319	17.690	-2.032	75.694	0.50	38.96	AC1
	ATOM	831	CG	PRO	319	16.927	-3.116	76.402	0.50	39.34	AC1
	ATOM	832	C	PRO	319	19.310	-2.080	73.756	0.50	35.85	AC1
15	ATOM	833	O	PRO	319	20.394	-2.240	74.319	0.50	35.73	AC1
	ATOM	834	N	PRO	320	19.197	-1.403	72.599	1.00	33.69	
	ATOM	835	CD	PRO	320	18.041	-1.404	71.692	1.00	32.09	
	ATOM	836	CA	PRO	320	20.362	-0.784	71.952	1.00	30.83	
	ATOM	837	CB	PRO	320	19.769	-0.083	70.722	1.00	30.11	
20	ATOM	838	CG	PRO	320	18.279	-0.174	70.892	1.00	32.74	
	ATOM	839	C	PRO	320	21.008	0.185	72.949	1.00	27.19	
	ATOM	840	O	PRO	320	20.317	0.824	73.756	1.00	27.36	
	ATOM	841	N	GLN	321	22.328	0.297	72.890	1.00	25.76	
	ATOM	842	CA	GLN	321	23.060	1.121	73.847	1.00	25.85	
25	ATOM	843	CB	GLN	321	24.262	0.329	74.357	1.00	29.20	
	ATOM	844	CG	GLN	321	23.925	-1.090	74.757	1.00	34.12	
	ATOM	845	CD	GLN	321	23.408	-1.197	76.163	1.00	38.11	
	ATOM	846	OE1	GLN	321	24.127	-0.916	77.123	1.00	40.85	
	ATOM	847	NE2	GLN	321	22.150	-1.617	76.302	1.00	40.57	
30	ATOM	848	C	GLN	321	23.546	2.495	73.423	1.00	23.90	
	ATOM	849	O	GLN	321	23.914	3.297	74.275	1.00	24.18	
	ATOM	850	N	LEU	322	23.536	2.790	72.128	1.00	22.59	
	ATOM	851	CA	LEU	322	24.050	4.080	71.666	1.00	21.41	
	ATOM	852	CB	LEU	322	25.291	3.879	70.775	1.00	22.86	
35	ATOM	853	CG	LEU	322	26.560	3.362	71.432	1.00	25.45	
	ATOM	854	CD1	LEU	322	27.625	3.130	70.345	1.00	28.06	

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	ATOM	855	CD2	LEU	322	27.036	4.384	72.497	1.00	24.21
	ATOM	856	C	LEU	322	23.079	4.942	70.891	1.00	22.08
	ATOM	857	O	LEU	322	22.435	4.478	69.961	1.00	23.11
	ATOM	858	N	MET	323	23.003	6.205	71.270	1.00	20.81
5	ATOM	859	CA	MET	323	22.145	7.157	70.590	1.00	21.91
	ATOM	860	CB	MET	323	21.213	7.835	71.598	1.00	23.20
	ATOM	861	CG	MET	323	20.325	8.922	70.978	1.00	22.36
	ATOM	862	SD	MET	323	19.196	9.636	72.187	1.00	22.04
	ATOM	863	CE	MET	323	18.026	8.314	72.302	1.00	22.12
10	ATOM	864	C	MET	323	23.054	8.187	69.914	1.00	25.54
	ATOM	865	O	MET	323	24.002	8.691	70.530	1.00	25.31
	ATOM	866	N	CYS	324	22.781	8.506	68.650	1.00	22.41
	ATOM	867	CA	CYS	324	23.619	9.483	67.941	1.00	24.83
	ATOM	868	CB	CYS	324	23.854	9.029	66.512	1.00	23.91
15	ATOM	869	SG	CYS	324	24.921	10.185	65.588	1.00	27.74
	ATOM	870	C	CYS	324	22.995	10.873	67.950	1.00	24.34
	ATOM	871	O	CYS	324	22.010	11.148	67.249	1.00	24.90
	ATOM	872	N	LEU	325	23.560	11.758	68.749	1.00	24.49
	ATOM	873	CA	LEU	325	23.038	13.114	68.843	1.00	25.66
20	ATOM	874	CB	LEU	325	23.421	13.746	70.183	1.00	26.79
	ATOM	875	CG	LEU	325	22.935	12.964	71.421	1.00	27.19
	ATOM	876	CD1	LEU	325	23.256	13.744	72.704	1.00	29.28
	ATOM	877	CD2	LEU	325	21.423	12.732	71.320	1.00	27.92
	ATOM	878	C	LEU	325	23.513	13.990	67.682	1.00	28.10
25	ATOM	879	O	LEU	325	22.860	14.978	67.344	1.00	31.20
	ATOM	880	N	MET	326	24.650	13.618	67.094	1.00	28.83
	ATOM	881	CA	MET	326	25.253	14.311	65.947	1.00	30.95
	ATOM	882	CB	MET	326	25.726	15.721	66.350	1.00	31.86
	ATOM	883	CG	MET	326	26.894	15.710	67.335	1.00	31.84
30	ATOM	884	SD	MET	326	27.648	17.333	67.693	1.00	34.98
	ATOM	885	CE	MET	326	29.085	16.800	68.706	1.00	30.77
	ATOM	886	C	MET	326	26.462	13.453	65.513	1.00	33.06
	ATOM	887	O	MET	326	26.882	12.565	66.242	1.00	32.71
	ATOM	888	N	PRO	327	27.013	13.682	64.307	1.00	35.54
35	ATOM	889	CD	PRO	327	26.511	14.545	63.227	1.00	35.87
	ATOM	890	CA	PRO	327	28.180	12.896	63.857	1.00	36.24

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	ATOM	891	CB	PRO	327	28.508	13.519	62.503	1.00	37.87
	ATOM	892	CG	PRO	327	27.159	13.932	62.001	1.00	35.11
	ATOM	893	C	PRO	327	29.353	13.035	64.836	1.00	38.75
	ATOM	894	O	PRO	327	29.754	14.154	65.155	1.00	38.99
5	ATOM	895	N	GLY	328	29.890	11.908	65.314	1.00	38.52
	ATOM	896	CA	GLY	328	31.001	11.933	66.257	1.00	38.65
	ATOM	897	C	GLY	328	30.606	12.217	67.700	1.00	38.39
	ATOM	898	O	GLY	328	31.431	12.604	68.545	1.00	39.05
	ATOM	899	N	MET	329	29.326	12.020	67.994	1.00	36.32
10	ATOM	900	CA	MET	329	28.830	12.251	69.326	1.00	34.24
	ATOM	901	CB	MET	329	28.343	13.693	69.451	1.00	38.91
	ATOM	902	CG	MET	329	27.462	13.991	70.649	1.00	44.24
	ATOM	903	SD	MET	329	28.233	13.696	72.235	1.00	50.95
	ATOM	904	CE	MET	329	26.854	12.835	73.089	1.00	48.58
15	ATOM	905	C	MET	329	27.700	11.271	69.603	1.00	30.52
	ATOM	906	O	MET	329	26.647	11.331	68.975	1.00	28.92
	ATOM	907	N	THR	330	27.960	10.324	70.490	1.00	26.42
	ATOM	908	CA	THR	330	26.933	9.370	70.865	1.00	23.65
	ATOM	909	CB	THR	330	27.338	7.895	70.542	1.00	24.12
20	ATOM	910	OG1	THR	330	28.672	7.654	71.005	1.00	27.18
	ATOM	911	CG2	THR	330	27.269	7.622	69.034	1.00	26.34
	ATOM	912	C	THR	330	26.685	9.475	72.360	1.00	23.23
	ATOM	913	O	THR	330	27.572	9.802	73.146	1.00	23.91
	ATOM	914	N	LEU	331	25.450	9.211	72.748	1.00	20.37
25	ATOM	915	CA	LEU	331	25.082	9.213	74.142	1.00	21.33
	ATOM	916	CB	LEU	331	23.773	9.986	74.340	1.00	24.38
	ATOM	917	CG	LEU	331	23.113	9.731	75.696	1.00	25.70
	ATOM	918	CD1	LEU	331	23.979	10.317	76.825	1.00	30.48
	ATOM	919	CD2	LEU	331	21.723	10.348	75.694	1.00	29.64
30	ATOM	920	C	LEU	331	24.892	7.737	74.489	1.00	21.13
	ATOM	921	O	LEU	331	24.158	7.026	73.819	1.00	19.21
	ATOM	922	N	HIS	332	25.582	7.262	75.525	1.00	18.80
	ATOM	923	CA	HIS	332	25.472	5.864	75.901	1.00	18.64
	ATOM	924	CB	HIS	332	26.740	5.417	76.658	1.00	18.77
35	ATOM	925	CG	HIS	332	26.826	3.938	76.862	1.00	21.68
	ATOM	926	CD2	HIS	332	27.533	2.991	76.205	1.00	22.97

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	ATOM	927	ND1	HIS	332	26.092	3.273	77.824	1.00	22.38
	ATOM	928	CE1	HIS	332	26.340	1.978	77.745	1.00	23.74
	ATOM	929	NE2	HIS	332	27.213	1.778	76.769	1.00	25.26
	ATOM	930	C	HIS	332	24.262	5.721	76.820	1.00	18.95
5	ATOM	931	O	HIS	332	23.981	6.620	77.616	1.00	19.91
	ATOM	932	N	ARG	333	23.594	4.581	76.715	1.00	19.39
	ATOM	933	CA	ARG	333	22.394	4.282	77.509	1.00	19.71
	ATOM	934	CB	ARG	333	21.930	2.850	77.235	1.00	20.65
	ATOM	935	CG	ARG	333	20.582	2.512	77.896	1.00	21.54
10	ATOM	936	CD	ARG	333	20.018	1.212	77.353	1.00	21.69
	ATOM	937	NE	ARG	333	18.703	0.862	77.899	1.00	20.98
	ATOM	938	CZ	ARG	333	18.501	0.034	78.921	1.00	22.46
	ATOM	939	NH1	ARG	333	19.535	-0.547	79.531	1.00	24.12
	ATOM	940	NH2	ARG	333	17.255	-0.241	79.309	1.00	20.87
15	ATOM	941	C	ARG	333	22.643	4.463	79.018	1.00	21.14
	ATOM	942	O	ARG	333	21.782	4.926	79.755	1.00	18.39
	ATOM	943	N	ASN	334	23.832	4.107	79.484	1.00	21.27
	ATOM	944	CA	ASN	334	24.114	4.259	80.910	1.00	23.47
	ATOM	945	CB	ASN	334	25.486	3.653	81.244	1.00	24.93
20	ATOM	946	CG	ASN	334	25.504	2.119	81.158	1.00	25.59
	ATOM	947	OD1	ASN	334	24.467	1.461	81.054	1.00	26.24
	ATOM	948	ND2	ASN	334	26.707	1.544	81.204	1.00	29.08
	ATOM	949	C	ASN	334	24.048	5.718	81.380	1.00	22.91
	ATOM	950	O	ASN	334	23.649	6.000	82.530	1.00	22.99
25	ATOM	951	N	SER	335	24.441	6.657	80.524	1.00	22.89
	ATOM	952	CA	SER	335	24.378	8.059	80.904	1.00	22.41
	ATOM	953	CB	SER	335	25.178	8.915	79.930	1.00	27.35
	ATOM	954	OG	SER	335	26.517	8.437	79.856	1.00	31.39
	ATOM	955	C	SER	335	22.908	8.484	80.939	1.00	23.03
30	ATOM	956	O	SER	335	22.496	9.260	81.809	1.00	22.21
	ATOM	957	N	ALA	336	22.126	7.970	79.989	1.00	21.81
	ATOM	958	CA	ALA	336	20.703	8.255	79.952	1.00	21.09
	ATOM	959	CB	ALA	336	20.060	7.595	78.718	1.00	21.81
	ATOM	960	C	ALA	336	20.044	7.744	81.232	1.00	21.37
35	ATOM	961	O	ALA	336	19.209	8.425	81.830	1.00	19.40
	ATOM	962	N	LEU	337	20.423	6.540	81.660	1.00	19.77

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	ATOM	963	CA	LEU	337	19.860	5.960	82.865	1.00	19.59
	ATOM	964	CB	LEU	337	20.374	4.517	83.039	1.00	19.20
	ATOM	965	CG	LEU	337	19.835	3.502	82.031	1.00	20.97
	ATOM	966	CD1	LEU	337	20.702	2.280	82.055	1.00	23.49
5	ATOM	967	CD2	LEU	337	18.391	3.164	82.329	1.00	21.07
	ATOM	968	C	LEU	337	20.206	6.777	84.089	1.00	20.54
	ATOM	969	O	LEU	337	19.364	6.997	84.985	1.00	19.57
	ATOM	970	N	GLN	338	21.454	7.226	84.131	1.00	21.36
	ATOM	971	CA	GLN	338	21.920	7.994	85.264	1.00	22.39
10	ATOM	972	CB	GLN	338	23.439	8.206	85.179	1.00	22.44
	ATOM	973	CG	GLN	338	23.973	8.755	86.488	1.00	27.14
	ATOM	974	CD	GLN	338	25.467	9.026	86.481	1.00	29.23
	ATOM	975	OE1	GLN	338	25.955	9.827	87.278	1.00	30.73
	ATOM	976	NE2	GLN	338	26.196	8.360	85.596	1.00	30.79
15	ATOM	977	C	GLN	338	21.200	9.331	85.381	1.00	23.40
	ATOM	978	O	GLN	338	20.894	9.790	86.490	1.00	21.75
	ATOM	979	N	ALA	339	20.899	9.935	84.227	1.00	22.63
	ATOM	980	CA	ALA	339	20.215	11.217	84.191	1.00	24.41
	ATOM	981	CB	ALA	339	20.430	11.903	82.832	1.00	23.46
20	ATOM	982	C	ALA	339	18.727	11.082	84.463	1.00	24.73
	ATOM	983	O	ALA	339	18.059	12.084	84.641	1.00	27.16
	ATOM	984	N	GLY	340	18.218	9.850	84.499	1.00	22.58
	ATOM	985	CA	GLY	340	16.803	9.622	84.754	1.00	23.89
	ATOM	986	C	GLY	340	15.898	9.580	83.531	1.00	25.09
25	ATOM	987	O	GLY	340	14.666	9.607	83.666	1.00	25.54
	ATOM	988	N	VAL	341	16.492	9.479	82.346	1.00	23.51
	ATOM	989	CA	VAL	341	15.719	9.473	81.095	1.00	20.92
	ATOM	990	CB	VAL	341	16.134	10.677	80.211	1.00	21.83
	ATOM	991	CG1	VAL	341	15.838	11.981	80.942	1.00	21.94
30	ATOM	992	CG2	VAL	341	17.621	10.577	79.858	1.00	21.91
	ATOM	993	C	VAL	341	15.891	8.185	80.300	1.00	20.24
	ATOM	994	O	VAL	341	15.803	8.182	79.083	1.00	19.53
	ATOM	995	N	GLY	342	16.132	7.079	80.999	1.00	19.65
	ATOM	996	CA	GLY	342	16.324	5.827	80.301	1.00	18.76
35	ATOM	997	C	GLY	342	15.104	5.352	79.541	1.00	19.27
	ATOM	998	O	GLY	342	15.230	4.771	78.470	1.00	18.82

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	ATOM	999	N	GLN	343	13.922	5.598	80.088	0.50	18.31	AC1
	ATOM	1000	CA	GLN	343	12.706	5.163	79.422	0.50	19.11	AC1
	ATOM	1001	CB	GLN	343	11.507	5.485	80.305	0.50	19.94	AC1
	ATOM	1002	CG	GLN	343	10.200	4.866	79.867	0.50	22.91	AC1
5	ATOM	1003	CD	GLN	343	9.082	5.177	80.852	0.50	24.13	AC1
	ATOM	1004	OE1	GLN	343	8.669	6.326	80.995	0.50	26.85	AC1
	ATOM	1005	NE2	GLN	343	8.606	4.154	81.555	0.50	25.40	AC1
	ATOM	1006	C	GLN	343	12.542	5.813	78.043	0.50	19.14	AC1
	ATOM	1007	O	GLN	343	12.318	5.127	77.050	0.50	18.83	AC1
10	ATOM	1008	N	ILE	344	12.664	7.136	77.977	1.00	17.95	
	ATOM	1009	CA	ILE	344	12.506	7.812	76.693	1.00	17.74	
	ATOM	1010	CB	ILE	344	12.348	9.372	76.875	1.00	18.47	
	ATOM	1011	CG2	ILE	344	13.700	10.010	77.231	1.00	20.66	
	ATOM	1012	CG1	ILE	344	11.754	9.984	75.596	1.00	19.04	
15	ATOM	1013	CD1	ILE	344	11.445	11.499	75.662	1.00	21.07	
	ATOM	1014	C	ILE	344	13.641	7.448	75.718	1.00	17.34	
	ATOM	1015	O	ILE	344	13.440	7.389	74.499	1.00	16.12	
	ATOM	1016	N	PHE	345	14.844	7.210	76.248	1.00	16.60	
	ATOM	1017	CA	PHE	345	15.976	6.826	75.417	1.00	17.63	
20	ATOM	1018	CB	PHE	345	17.208	6.636	76.322	1.00	17.86	
	ATOM	1019	CG	PHE	345	18.455	6.189	75.613	1.00	18.24	
	ATOM	1020	CD1	PHE	345	18.657	4.848	75.273	1.00	18.20	
	ATOM	1021	CD2	PHE	345	19.470	7.090	75.363	1.00	20.10	
	ATOM	1022	CE1	PHE	345	19.854	4.412	74.706	1.00	19.01	
25	ATOM	1023	CE2	PHE	345	20.663	6.673	74.798	1.00	17.96	
	ATOM	1024	CZ	PHE	345	20.861	5.328	74.469	1.00	18.58	
	ATOM	1025	C	PHE	345	15.603	5.522	74.710	1.00	18.98	
	ATOM	1026	O	PHE	345	15.756	5.389	73.491	1.00	18.15	
	ATOM	1027	N	ASP	346	15.072	4.568	75.480	1.00	18.04	
30	ATOM	1028	CA	ASP	346	14.695	3.300	74.894	1.00	18.83	
	ATOM	1029	CB	ASP	346	14.285	2.302	75.988	1.00	19.96	
	ATOM	1030	CG	ASP	346	15.467	1.768	76.786	1.00	24.04	
	ATOM	1031	OD1	ASP	346	16.630	2.038	76.430	1.00	24.95	
	ATOM	1032	OD2	ASP	346	15.232	1.043	77.784	1.00	24.86	
35	ATOM	1033	C	ASP	346	13.550	3.462	73.872	1.00	18.04	
	ATOM	1034	O	ASP	346	13.549	2.782	72.841	1.00	19.39	

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5	ATOM	1035	N	ARG	347	12.603	4.359	74.138	1.00	19.77
	ATOM	1036	CA	ARG	347	11.493	4.579	73.188	1.00	20.42
	ATOM	1037	CB	ARG	347	10.443	5.558	73.708	1.00	24.20
	ATOM	1038	CG	ARG	347	9.527	5.024	74.786	1.00	26.30
	ATOM	1039	CD	ARG	347	8.310	5.929	74.937	1.00	28.76
10	ATOM	1040	NE	ARG	347	7.383	5.807	73.813	1.00	29.58
	ATOM	1041	CZ	ARG	347	6.312	6.577	73.629	1.00	31.91
	ATOM	1042	NH1	ARG	347	6.028	7.536	74.492	1.00	32.14
	ATOM	1043	NH2	ARG	347	5.522	6.378	72.579	1.00	32.47
	ATOM	1044	C	ARG	347	12.012	5.120	71.875	1.00	20.09
15	ATOM	1045	O	ARG	347	11.586	4.703	70.806	1.00	18.14
	ATOM	1046	N	VAL	348	12.939	6.073	71.945	1.00	18.48
	ATOM	1047	CA	VAL	348	13.480	6.621	70.708	1.00	18.94
	ATOM	1048	CB	VAL	348	14.532	7.713	70.991	1.00	18.19
	ATOM	1049	CG1	VAL	348	15.286	8.052	69.706	1.00	18.18
20	ATOM	1050	CG2	VAL	348	13.862	8.930	71.600	1.00	19.11
	ATOM	1051	C	VAL	348	14.143	5.518	69.882	1.00	18.63
	ATOM	1052	O	VAL	348	13.885	5.380	68.691	1.00	17.99
	ATOM	1053	N	LEU	349	14.981	4.709	70.514	1.00	18.35
	ATOM	1054	CA	LEU	349	15.679	3.686	69.749	1.00	19.38
25	ATOM	1055	CB	LEU	349	16.906	3.175	70.526	1.00	20.34
	ATOM	1056	CG	LEU	349	17.920	4.286	70.807	1.00	20.49
	ATOM	1057	CD1	LEU	349	19.173	3.626	71.408	1.00	23.32
	ATOM	1058	CD2	LEU	349	18.273	5.078	69.500	1.00	18.92
	ATOM	1059	C	LEU	349	14.822	2.509	69.294	1.00	20.39
30	ATOM	1060	O	LEU	349	15.112	1.901	68.263	1.00	19.62
	ATOM	1061	N	SER	350	13.746	2.208	70.025	1.00	21.15
	ATOM	1062	CA	SER	350	12.907	1.074	69.623	1.00	23.27
	ATOM	1063	CB	SER	350	12.443	0.294	70.855	1.00	25.65
	ATOM	1064	OG	SER	350	11.622	1.081	71.687	1.00	28.64
35	ATOM	1065	C	SER	350	11.698	1.451	68.766	1.00	21.84
	ATOM	1066	O	SER	350	11.424	0.790	67.762	1.00	25.35
	ATOM	1067	N	GLU	351	10.986	2.516	69.131	1.00	22.62
	ATOM	1068	CA	GLU	351	9.801	2.906	68.368	1.00	22.04
	ATOM	1069	CB	GLU	351	8.834	3.680	69.252	1.00	22.43
	ATOM	1070	CG	GLU	351	8.454	2.916	70.486	1.00	26.86

	ATOM	1071	CD	GLU	351	7.434	3.650	71.303	1.00	28.97	
	ATOM	1072	OE1	GLU	351	7.473	3.544	72.548	1.00	31.85	
	ATOM	1073	OE2	GLU	351	6.581	4.330	70.691	1.00	32.68	
	ATOM	1074	C	GLU	351	10.133	3.708	67.132	1.00	22.11	
5	ATOM	1075	O	GLU	351	9.348	3.766	66.183	1.00	22.30	
	ATOM	1076	N	LEU	352	11.309	4.328	67.113	1.00	19.99	
	ATOM	1077	CA	LEU	352	11.696	5.083	65.934	1.00	19.01	
	ATOM	1078	CB	LEU	352	12.043	6.555	66.293	1.00	18.64	
	ATOM	1079	CG	LEU	352	10.911	7.365	66.950	1.00	19.12	
10	ATOM	1080	CD1	LEU	352	11.445	8.742	67.339	1.00	19.51	
	ATOM	1081	CD2	LEU	352	9.703	7.505	66.018	1.00	19.25	
	ATOM	1082	C	LEU	352	12.859	4.467	65.163	1.00	19.51	
	ATOM	1083	O	LEU	352	12.704	3.977	64.038	1.00	21.10	
	ATOM	1084	N	SER	353	14.052	4.464	65.754	0.50	18.72	AC1
15	ATOM	1085	CA	SER	353	15.203	3.933	65.034	0.50	18.55	AC1
	ATOM	1086	CB	SER	353	16.473	4.032	65.883	0.50	16.66	AC1
	ATOM	1087	OG	SER	353	16.782	5.378	66.160	0.50	11.47	AC1
	ATOM	1088	C	SER	353	15.045	2.500	64.546	0.50	19.60	AC1
	ATOM	1089	O	SER	353	15.207	2.236	63.355	0.50	20.26	AC1
20	ATOM	1090	N	LEU	354	14.746	1.579	65.455	1.00	21.67	
	ATOM	1091	CA	LEU	354	14.602	0.181	65.051	1.00	23.55	
	ATOM	1092	CB	LEU	354	14.360	-0.715	66.278	1.00	24.35	
	ATOM	1093	CG	LEU	354	14.284	-2.222	66.012	1.00	30.18	
	ATOM	1094	CD1	LEU	354	15.388	-2.664	65.055	1.00	31.88	
25	ATOM	1095	CD2	LEU	354	14.392	-2.944	67.345	1.00	31.36	
	ATOM	1096	C	LEU	354	13.489	-0.011	64.009	1.00	24.82	
	ATOM	1097	O	LEU	354	13.696	-0.684	63.004	1.00	25.66	
	ATOM	1098	N	LYS	355	12.324	0.587	64.234	1.00	26.97	
	ATOM	1099	CA	LYS	355	11.236	0.454	63.272	1.00	26.95	
30	ATOM	1100	CB	LYS	355	10.003	1.226	63.735	1.00	29.30	
	ATOM	1101	CG	LYS	355	9.228	0.572	64.843	1.00	34.34	
	ATOM	1102	CD	LYS	355	8.440	-0.616	64.321	1.00	38.57	
	ATOM	1103	CE	LYS	355	7.365	-1.007	65.319	1.00	39.54	
	ATOM	1104	NZ	LYS	355	7.883	-0.958	66.713	1.00	40.20	
35	ATOM	1105	C	LYS	355	11.637	0.964	61.899	1.00	27.30	
	ATOM	1106	O	LYS	355	11.281	0.369	60.883	1.00	28.58	

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	ATOM	1107	N	MET	356	12.362	2.080	61.860	1.00	25.41
	ATOM	1108	CA	MET	356	12.787	2.641	60.594	1.00	25.37
	ATOM	1109	CB	MET	356	13.279	4.071	60.778	1.00	27.04
	ATOM	1110	CG	MET	356	12.126	5.017	60.918	1.00	26.57
5	ATOM	1111	SD	MET	356	12.669	6.671	60.768	1.00	36.72
	ATOM	1112	CE	MET	356	13.015	6.835	62.357	1.00	16.80
	ATOM	1113	C	MET	356	13.836	1.808	59.896	1.00	26.93
	ATOM	1114	O	MET	356	13.907	1.807	58.676	1.00	25.41
	ATOM	1115	N	ARG	357	14.672	1.114	60.661	1.00	27.88
10	ATOM	1116	CA	ARG	357	15.656	0.281	60.003	1.00	29.75
	ATOM	1117	CB	ARG	357	16.733	-0.214	60.961	1.00	31.09
	ATOM	1118	CG	ARG	357	17.748	-1.056	60.213	1.00	35.17
	ATOM	1119	CD	ARG	357	18.840	-1.607	61.112	1.00	38.46
	ATOM	1120	NE	ARG	357	18.313	-2.543	62.097	1.00	41.53
15	ATOM	1121	CZ	ARG	357	19.066	-3.164	63.003	1.00	43.38
	ATOM	1122	NH1	ARG	357	20.376	-2.942	63.037	1.00	42.92
	ATOM	1123	NH2	ARG	357	18.512	-3.995	63.879	1.00	43.48
	ATOM	1124	C	ARG	357	14.926	-0.925	59.422	1.00	29.63
	ATOM	1125	O	ARG	357	15.218	-1.353	58.310	1.00	29.83
20	ATOM	1126	N	THR	358	13.966	-1.452	60.171	1.00	29.51
	ATOM	1127	CA	THR	358	13.204	-2.609	59.704	1.00	30.65
	ATOM	1128	CB	THR	358	12.273	-3.117	60.812	1.00	31.00
	ATOM	1129	OG1	THR	358	13.071	-3.609	61.895	1.00	32.46
	ATOM	1130	CG2	THR	358	11.374	-4.260	60.306	1.00	34.28
25	ATOM	1131	C	THR	358	12.408	-2.281	58.438	1.00	30.73
	ATOM	1132	O	THR	358	12.286	-3.114	57.533	1.00	32.33
	ATOM	1133	N	LEU	359	11.895	-1.056	58.359	1.00	29.40
	ATOM	1134	CA	LEU	359	11.124	-0.610	57.201	1.00	29.68
	ATOM	1135	CB	LEU	359	10.242	0.583	57.605	1.00	30.32
30	ATOM	1136	CG	LEU	359	8.732	0.609	57.321	1.00	34.26
	ATOM	1137	CD1	LEU	359	8.197	2.038	57.529	1.00	33.77
	ATOM	1138	CD2	LEU	359	8.452	0.142	55.900	1.00	34.08
	ATOM	1139	C	LEU	359	12.046	-0.168	56.066	1.00	28.77
	ATOM	1140	O	LEU	359	11.585	0.164	54.974	1.00	27.98
35	ATOM	1141	N	ARG	360	13.349	-0.130	56.327	1.00	30.53
	ATOM	1142	CA	ARG	360	14.315	0.310	55.327	1.00	30.15

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	ATOM	1143	CB	ARG	360	14.381	-0.695	54.178	1.00	33.80
	ATOM	1144	CG	ARG	360	14.798	-2.076	54.625	1.00	36.43
	ATOM	1145	CD	ARG	360	14.018	-3.165	53.900	1.00	39.56
	ATOM	1146	NE	ARG	360	12.588	-3.168	54.226	1.00	41.14
5	ATOM	1147	CZ	ARG	360	11.618	-2.942	53.340	1.00	42.18
	ATOM	1148	NH1	ARG	360	11.918	-2.688	52.071	1.00	41.02
	ATOM	1149	NH2	ARG	360	10.345	-2.983	53.717	1.00	42.86
	ATOM	1150	C	ARG	360	13.975	1.699	54.787	1.00	29.92
	ATOM	1151	O	ARG	360	14.073	1.958	53.592	1.00	28.84
10	ATOM	1152	N	VAL	361	13.569	2.600	55.677	1.00	27.64
	ATOM	1153	CA	VAL	361	13.261	3.956	55.267	1.00	25.17
	ATOM	1154	CB	VAL	361	12.909	4.819	56.480	1.00	24.00
	ATOM	1155	CG1	VAL	361	12.684	6.254	56.066	1.00	24.37
	ATOM	1156	CG2	VAL	361	11.688	4.249	57.166	1.00	23.19
15	ATOM	1157	C	VAL	361	14.504	4.525	54.594	1.00	25.34
	ATOM	1158	O	VAL	361	15.613	4.407	55.133	1.00	25.79
	ATOM	1159	N	ASP	362	14.344	5.109	53.404	1.00	24.62
	ATOM	1160	CA	ASP	362	15.481	5.712	52.718	1.00	24.80
	ATOM	1161	CB	ASP	362	15.540	5.316	51.223	1.00	27.01
20	ATOM	1162	CG	ASP	362	14.307	5.720	50.433	1.00	29.25
	ATOM	1163	OD1	ASP	362	13.697	6.764	50.731	1.00	27.58
	ATOM	1164	OD2	ASP	362	13.963	4.987	49.479	1.00	32.41
	ATOM	1165	C	ASP	362	15.520	7.226	52.863	1.00	25.99
	ATOM	1166	O	ASP	362	14.631	7.823	53.486	1.00	25.65
25	ATOM	1167	N	GLN	363	16.561	7.845	52.312	1.00	24.73
	ATOM	1168	CA	GLN	363	16.742	9.286	52.405	1.00	26.50
	ATOM	1169	CB	GLN	363	18.044	9.682	51.690	1.00	31.84
	ATOM	1170	CG	GLN	363	18.339	11.179	51.662	1.00	36.89
	ATOM	1171	CD	GLN	363	19.008	11.689	52.921	1.00	40.13
30	ATOM	1172	OE1	GLN	363	18.615	11.346	54.047	1.00	42.87
	ATOM	1173	NE2	GLN	363	20.013	12.536	52.743	1.00	40.44
	ATOM	1174	C	GLN	363	15.540	10.070	51.855	1.00	25.17
	ATOM	1175	O	GLN	363	15.077	11.020	52.480	1.00	22.69
	ATOM	1176	N	ALA	364	15.023	9.659	50.701	1.00	24.53
35	ATOM	1177	CA	ALA	364	13.863	10.340	50.099	1.00	22.80
	ATOM	1178	CB	ALA	364	13.524	9.691	48.753	1.00	22.91

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	ATOM	1179	C	ALA	364	12.631	10.326	51.022	1.00	21.81
	ATOM	1180	O	ALA	364	11.946	11.336	51.178	1.00	21.88
	ATOM	1181	N	GLU	365	12.362	9.188	51.636	1.00	22.72
	ATOM	1182	CA	GLU	365	11.218	9.062	52.532	1.00	21.63
5	ATOM	1183	CB	GLU	365	10.990	7.585	52.856	1.00	22.68
	ATOM	1184	CG	GLU	365	10.724	6.806	51.583	1.00	23.15
	ATOM	1185	CD	GLU	365	10.797	5.303	51.723	1.00	28.04
	ATOM	1186	OE1	GLU	365	11.632	4.813	52.501	1.00	26.39
	ATOM	1187	OE2	GLU	365	10.034	4.607	51.010	1.00	27.63
10	ATOM	1188	C	GLU	365	11.454	9.881	53.798	1.00	22.43
	ATOM	1189	O	GLU	365	10.557	10.570	54.298	1.00	22.18
	ATOM	1190	N	TYR	366	12.681	9.822	54.304	1.00	22.10
	ATOM	1191	CA	TYR	366	13.026	10.580	55.506	1.00	22.15
	ATOM	1192	CB	TYR	366	14.494	10.316	55.871	1.00	22.04
15	ATOM	1193	CG	TYR	366	15.010	11.209	56.986	1.00	22.63
	ATOM	1194	CD1	TYR	366	14.580	11.030	58.307	1.00	21.87
	ATOM	1195	CE1	TYR	366	15.023	11.864	59.328	1.00	22.24
	ATOM	1196	CD2	TYR	366	15.903	12.246	56.715	1.00	20.88
	ATOM	1197	CE2	TYR	366	16.366	13.092	57.731	1.00	22.98
20	ATOM	1198	CZ	TYR	366	15.913	12.899	59.041	1.00	22.25
	ATOM	1199	OH	TYR	366	16.315	13.752	60.054	1.00	23.04
	ATOM	1200	C	TYR	366	12.797	12.095	55.332	1.00	19.98
	ATOM	1201	O	TYR	366	12.209	12.731	56.199	1.00	19.55
	ATOM	1202	N	VAL	367	13.260	12.676	54.225	1.00	20.09
25	ATOM	1203	CA	VAL	367	13.080	14.106	54.034	1.00	19.12
	ATOM	1204	CB	VAL	367	13.955	14.666	52.891	1.00	20.38
	ATOM	1205	CG1	VAL	367	15.446	14.473	53.249	1.00	21.37
	ATOM	1206	CG2	VAL	367	13.609	14.009	51.554	1.00	19.90
	ATOM	1207	C	VAL	367	11.607	14.458	53.784	1.00	18.65
30	ATOM	1208	O	VAL	367	11.165	15.538	54.178	1.00	18.48
	ATOM	1209	N	ALA	368	10.868	13.552	53.147	1.00	20.47
	ATOM	1210	CA	ALA	368	9.447	13.787	52.893	1.00	19.05
	ATOM	1211	CB	ALA	368	8.854	12.668	51.988	1.00	18.93
	ATOM	1212	C	ALA	368	8.714	13.813	54.240	1.00	19.17
35	ATOM	1213	O	ALA	368	7.863	14.682	54.487	1.00	18.81
	ATOM	1214	N	LEU	369	9.048	12.871	55.112	1.00	19.43

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	ATOM	1215	CA	LEU	369	8.417	12.819	56.428	1.00	17.85
	ATOM	1216	CB	LEU	369	8.807	11.526	57.147	1.00	20.14
	ATOM	1217	CG	LEU	369	8.153	10.250	56.565	1.00	21.25
	ATOM	1218	CD1	LEU	369	8.810	9.041	57.154	1.00	22.02
5	ATOM	1219	CD2	LEU	369	6.626	10.219	56.856	1.00	21.64
	ATOM	1220	C	LEU	369	8.772	14.076	57.235	1.00	19.07
	ATOM	1221	O	LEU	369	7.945	14.606	57.965	1.00	17.17
	ATOM	1222	N	LYS	370	10.007	14.567	57.120	1.00	18.01
	ATOM	1223	CA	LYS	370	10.363	15.799	57.826	1.00	19.26
10	ATOM	1224	CB	LYS	370	11.819	16.199	57.522	1.00	18.97
	ATOM	1225	CG	LYS	370	12.888	15.349	58.203	1.00	21.31
	ATOM	1226	CD	LYS	370	14.304	15.860	57.845	1.00	25.49
	ATOM	1227	CE	LYS	370	14.445	17.367	58.009	1.00	25.79
	ATOM	1228	NZ	LYS	370	15.878	17.841	57.879	1.00	29.87
15	ATOM	1229	C	LYS	370	9.440	16.949	57.388	1.00	17.68
	ATOM	1230	O	LYS	370	8.950	17.717	58.203	1.00	17.05
	ATOM	1231	N	ALA	371	9.209	17.075	56.081	1.00	17.98
	ATOM	1232	CA	ALA	371	8.368	18.154	55.596	1.00	17.26
	ATOM	1233	CB	ALA	371	8.344	18.154	54.065	1.00	19.00
20	ATOM	1234	C	ALA	371	6.957	17.957	56.140	1.00	15.65
	ATOM	1235	O	ALA	371	6.299	18.909	56.533	1.00	17.13
	ATOM	1236	N	ILE	372	6.492	16.713	56.151	1.00	14.92
	ATOM	1237	CA	ILE	372	5.146	16.450	56.673	1.00	16.38
	ATOM	1238	CB	ILE	372	4.743	14.956	56.430	1.00	15.28
25	ATOM	1239	CG2	ILE	372	3.477	14.602	57.245	1.00	17.98
	ATOM	1240	CG1	ILE	372	4.566	14.730	54.915	1.00	18.14
	ATOM	1241	CD1	ILE	372	4.413	13.271	54.530	1.00	18.13
	ATOM	1242	C	ILE	372	5.038	16.795	58.163	1.00	16.98
	ATOM	1243	O	ILE	372	4.028	17.317	58.606	1.00	16.87
30	ATOM	1244	N	ILE	373	6.089	16.522	58.942	1.00	14.47
	ATOM	1245	CA	ILE	373	6.080	16.829	60.369	1.00	15.13
	ATOM	1246	CB	ILE	373	7.392	16.251	61.042	1.00	13.81
	ATOM	1247	CG2	ILE	373	7.530	16.783	62.463	1.00	15.08
	ATOM	1248	CG1	ILE	373	7.340	14.717	61.052	1.00	14.66
35	ATOM	1249	CD1	ILE	373	8.709	14.031	61.219	1.00	17.60
	ATOM	1250	C	ILE	373	5.962	18.350	60.604	1.00	15.01

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	ATOM	1251	O	ILE	373	5.212	18.817	61.477	1.00	15.67
	ATOM	1252	N	LEU	374	6.702	19.109	59.796	1.00	16.23
	ATOM	1253	CA	LEU	374	6.688	20.557	59.880	1.00	15.91
	ATOM	1254	CB	LEU	374	7.738	21.160	58.942	1.00	18.27
5	ATOM	1255	CG	LEU	374	7.702	22.700	58.759	1.00	19.49
	ATOM	1256	CD1	LEU	374	8.184	23.403	60.044	1.00	18.70
	ATOM	1257	CD2	LEU	374	8.596	23.092	57.597	1.00	19.61
	ATOM	1258	C	LEU	374	5.316	21.128	59.490	1.00	17.14
	ATOM	1259	O	LEU	374	4.765	21.980	60.167	1.00	16.72
10	ATOM	1260	N	LEU	375	4.803	20.662	58.367	1.00	17.78
	ATOM	1261	CA	LEU	375	3.561	21.202	57.831	1.00	17.01
	ATOM	1262	CB	LEU	375	3.573	21.071	56.301	1.00	19.06
	ATOM	1263	CG	LEU	375	4.788	21.715	55.581	1.00	18.84
	ATOM	1264	CD1	LEU	375	4.903	21.197	54.151	1.00	18.22
15	ATOM	1265	CD2	LEU	375	4.644	23.234	55.610	1.00	19.41
	ATOM	1266	C	LEU	375	2.349	20.514	58.422	1.00	19.26
	ATOM	1267	O	LEU	375	1.603	19.823	57.705	1.00	19.50
	ATOM	1268	N	ASN	376	2.178	20.727	59.723	1.00	16.95
	ATOM	1269	CA	ASN	376	1.087	20.136	60.510	1.00	19.78
20	ATOM	1270	CB	ASN	376	1.605	19.772	61.912	1.00	18.97
	ATOM	1271	CG	ASN	376	0.537	19.124	62.780	1.00	23.13
	ATOM	1272	OD1	ASN	376	-0.527	18.732	62.289	1.00	19.72
	ATOM	1273	ND2	ASN	376	0.827	18.989	64.081	1.00	21.10
	ATOM	1274	C	ASN	376	-0.088	21.080	60.641	1.00	17.80
25	ATOM	1275	O	ASN	376	-0.043	22.028	61.412	1.00	18.77
	ATOM	1276	N	PRO	377	-1.188	20.820	59.909	1.00	20.03
	ATOM	1277	CD	PRO	377	-1.463	19.684	59.010	1.00	19.34
	ATOM	1278	CA	PRO	377	-2.342	21.728	60.011	1.00	20.40
	ATOM	1279	CB	PRO	377	-3.239	21.293	58.858	1.00	18.78
30	ATOM	1280	CG	PRO	377	-2.979	19.796	58.774	1.00	19.22
	ATOM	1281	C	PRO	377	-3.086	21.705	61.336	1.00	21.89
	ATOM	1282	O	PRO	377	-3.922	22.583	61.594	1.00	22.57
	ATOM	1283	N	ASP	378	-2.771	20.723	62.177	1.00	20.09
	ATOM	1284	CA	ASP	378	-3.444	20.609	63.463	1.00	22.47
35	ATOM	1285	CB	ASP	378	-3.608	19.131	63.809	1.00	23.71
	ATOM	1286	CG	ASP	378	-4.555	18.426	62.847	1.00	25.43

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	ATOM	1287	OD1 ASP	378	-5.579	19.028	62.487	1.00	28.35
	ATOM	1288	OD2 ASP	378	-4.289	17.283	62.443	1.00	30.58
	ATOM	1289	C ASP	378	-2.823	21.403	64.603	1.00	22.30
	ATOM	1290	O ASP	378	-3.265	21.309	65.760	1.00	22.98
5	ATOM	1291	N VAL	379	-1.793	22.181	64.279	1.00	22.51
	ATOM	1292	CA VAL	379	-1.167	23.053	65.266	1.00	21.52
	ATOM	1293	CB VAL	379	0.044	23.807	64.662	1.00	20.60
	ATOM	1294	CG1 VAL	379	0.424	25.004	65.532	1.00	22.27
	ATOM	1295	CG2 VAL	379	1.226	22.848	64.516	1.00	22.31
10	ATOM	1296	C VAL	379	-2.255	24.048	65.658	1.00	23.83
	ATOM	1297	O VAL	379	-2.918	24.655	64.793	1.00	25.06
	ATOM	1298	N LYS	380	-2.460	24.212	66.958	1.00	23.33
	ATOM	1299	CA LYS	380	-3.490	25.124	67.430	1.00	24.49
	ATOM	1300	CB LYS	380	-3.797	24.829	68.904	1.00	25.21
15	ATOM	1301	CG LYS	380	-4.182	23.365	69.131	1.00	28.03
	ATOM	1302	CD LYS	380	-4.460	23.035	70.594	1.00	30.82
	ATOM	1303	CE LYS	380	-4.728	21.536	70.758	1.00	31.68
	ATOM	1304	NZ LYS	380	-4.904	21.079	72.177	1.00	33.50
	ATOM	1305	C LYS	380	-3.055	26.573	67.250	1.00	24.85
20	ATOM	1306	O LYS	380	-1.874	26.891	67.408	1.00	25.55
	ATOM	1307	N GLY	381	-3.988	27.445	66.861	1.00	24.69
	ATOM	1308	CA GLY	381	-3.647	28.852	66.704	1.00	26.29
	ATOM	1309	C GLY	381	-3.384	29.378	65.295	1.00	25.30
	ATOM	1310	O GLY	381	-3.246	30.598	65.093	1.00	27.29
25	ATOM	1311	N LEU	382	-3.313	28.490	64.311	1.00	26.35
	ATOM	1312	CA LEU	382	-3.054	28.914	62.941	1.00	26.95
	ATOM	1313	CB LEU	382	-2.997	27.706	61.995	1.00	25.01
	ATOM	1314	CG LEU	382	-1.865	26.700	62.265	1.00	24.87
	ATOM	1315	CD1 LEU	382	-2.011	25.507	61.314	1.00	24.53
30	ATOM	1316	CD2 LEU	382	-0.518	27.384	62.064	1.00	24.40
	ATOM	1317	C LEU	382	-4.120	29.885	62.428	1.00	28.77
	ATOM	1318	O LEU	382	-5.310	29.719	62.695	1.00	28.39
	ATOM	1319	N LYS	383	-3.660	30.881	61.681	1.00	30.83
	ATOM	1320	CA LYS	383	-4.518	31.894	61.078	1.00	32.60
35	ATOM	1321	CB LYS	383	-3.670	33.104	60.699	1.00	35.65
	ATOM	1322	CG LYS	383	-4.352	34.121	59.788	1.00	40.31

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	ATOM	1323	CD	LYS	383	-5.044	35.203	60.589	1.00	42.92
	ATOM	1324	CE	LYS	383	-5.436	36.376	59.702	1.00	43.80
	ATOM	1325	NZ	LYS	383	-6.040	37.476	60.505	1.00	44.52
	ATOM	1326	C	LYS	383	-5.159	31.313	59.819	1.00	32.46
5	ATOM	1327	O	LYS	383	-6.374	31.411	59.620	1.00	33.42
	ATOM	1328	N	ASN	384	-4.332	30.700	58.977	1.00	30.19
	ATOM	1329	CA	ASN	384	-4.794	30.118	57.720	1.00	29.86
	ATOM	1330	CB	ASN	384	-4.154	30.854	56.549	1.00	32.74
	ATOM	1331	CG	ASN	384	-4.460	32.336	56.570	1.00	36.46
10	ATOM	1332	OD1	ASN	384	-5.625	32.730	56.585	1.00	39.59
	ATOM	1333	ND2	ASN	384	-3.418	33.166	56.583	1.00	37.88
	ATOM	1334	C	ASN	384	-4.466	28.636	57.636	1.00	26.29
	ATOM	1335	O	ASN	384	-3.558	28.229	56.912	1.00	26.38
	ATOM	1336	N	ARG	385	-5.218	27.845	58.387	1.00	24.62
15	ATOM	1337	CA	ARG	385	-5.005	26.406	58.431	1.00	24.85
	ATOM	1338	CB	ARG	385	-5.994	25.779	59.413	1.00	24.62
	ATOM	1339	CG	ARG	385	-5.910	24.275	59.561	1.00	27.77
	ATOM	1340	CD	ARG	385	-6.705	23.839	60.785	1.00	30.37
	ATOM	1341	NE	ARG	385	-5.976	24.188	62.004	1.00	31.78
20	ATOM	1342	CZ	ARG	385	-6.329	25.148	62.849	1.00	31.80
	ATOM	1343	NH1	ARG	385	-7.432	25.867	62.629	1.00	31.71
	ATOM	1344	NH2	ARG	385	-5.542	25.426	63.886	1.00	28.60
	ATOM	1345	C	ARG	385	-5.079	25.727	57.070	1.00	24.38
	ATOM	1346	O	ARG	385	-4.289	24.824	56.783	1.00	24.23
25	ATOM	1347	N	GLN	386	-6.003	26.165	56.214	1.00	24.39
	ATOM	1348	CA	GLN	386	-6.128	25.542	54.906	1.00	25.99
	ATOM	1349	CB	GLN	386	-7.320	26.124	54.128	1.00	29.68
	ATOM	1350	CG	GLN	386	-7.256	27.619	53.863	1.00	34.93
	ATOM	1351	CD	GLN	386	-7.246	28.442	55.136	1.00	37.35
30	ATOM	1352	OE1	GLN	386	-8.016	28.183	56.072	1.00	39.44
	ATOM	1353	NE2	GLN	386	-6.373	29.443	55.183	1.00	39.95
	ATOM	1354	C	GLN	386	-4.867	25.646	54.067	1.00	24.30
	ATOM	1355	O	GLN	386	-4.561	24.727	53.318	1.00	25.10
	ATOM	1356	N	GLU	387	-4.140	26.752	54.182	1.00	25.50
35	ATOM	1357	CA	GLU	387	-2.907	26.905	53.413	1.00	25.38
	ATOM	1358	CB	GLU	387	-2.358	28.328	53.594	1.00	29.21

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	ATOM	1359	CG	GLU	387	-3.234	29.420	52.915	1.00	33.12
	ATOM	1360	CD	GLU	387	-2.845	30.838	53.284	1.00	37.28
	ATOM	1361	OE1	GLU	387	-1.634	31.125	53.407	1.00	40.75
	ATOM	1362	OE2	GLU	387	-3.750	31.691	53.436	1.00	38.95
5	ATOM	1363	C	GLU	387	-1.877	25.841	53.852	1.00	25.54
	ATOM	1364	O	GLU	387	-1.097	25.329	53.030	1.00	24.67
	ATOM	1365	N	VAL	388	-1.897	25.476	55.132	1.00	24.28
	ATOM	1366	CA	VAL	388	-0.960	24.447	55.617	1.00	21.40
	ATOM	1367	CB	VAL	388	-0.845	24.439	57.168	1.00	19.68
10	ATOM	1368	CG1	VAL	388	0.182	23.410	57.597	1.00	22.22
	ATOM	1369	CG2	VAL	388	-0.477	25.824	57.691	1.00	20.28
	ATOM	1370	C	VAL	388	-1.444	23.076	55.178	1.00	22.10
	ATOM	1371	O	VAL	388	-0.666	22.211	54.782	1.00	21.10
	ATOM	1372	N	GLU	389	-2.750	22.859	55.243	1.00	22.00
15	ATOM	1373	CA	GLU	389	-3.284	21.577	54.825	1.00	21.41
	ATOM	1374	CB	GLU	389	-4.801	21.538	54.987	1.00	22.76
	ATOM	1375	CG	GLU	389	-5.358	20.146	54.988	1.00	31.47
	ATOM	1376	CD	GLU	389	-6.793	20.093	55.471	1.00	36.14
	ATOM	1377	OE1	GLU	389	-7.160	20.927	56.334	1.00	39.74
20	ATOM	1378	OE2	GLU	389	-7.540	19.204	55.006	1.00	39.63
	ATOM	1379	C	GLU	389	-2.936	21.294	53.382	1.00	19.32
	ATOM	1380	O	GLU	389	-2.653	20.155	53.025	1.00	21.32
	ATOM	1381	N	VAL	390	-3.001	22.313	52.534	1.00	19.72
	ATOM	1382	CA	VAL	390	-2.685	22.148	51.125	1.00	19.82
25	ATOM	1383	CB	VAL	390	-2.950	23.447	50.316	1.00	19.77
	ATOM	1384	CG1	VAL	390	-2.307	23.344	48.919	1.00	22.22
	ATOM	1385	CG2	VAL	390	-4.442	23.652	50.169	1.00	23.95
	ATOM	1386	C	VAL	390	-1.231	21.744	50.924	1.00	20.27
	ATOM	1387	O	VAL	390	-0.924	20.894	50.093	1.00	20.79
30	ATOM	1388	N	LEU	391	-0.334	22.345	51.699	1.00	21.06
	ATOM	1389	CA	LEU	391	1.078	22.004	51.552	1.00	19.84
	ATOM	1390	CB	LEU	391	1.951	22.982	52.328	1.00	20.90
	ATOM	1391	CG	LEU	391	1.895	24.438	51.836	1.00	21.65
	ATOM	1392	CD1	LEU	391	2.846	25.283	52.673	1.00	23.70
35	ATOM	1393	CD2	LEU	391	2.260	24.515	50.351	1.00	25.56
	ATOM	1394	C	LEU	391	1.327	20.583	52.031	1.00	19.59

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5	ATOM	1395	O	LEU	391	2.090	19.837	51.421	1.00	19.63	
	ATOM	1396	N	ARG	392	0.680	20.192	53.130	0.50	19.30	AC1
	ATOM	1397	CA	ARG	392	0.862	18.823	53.628	0.50	19.65	AC1
	ATOM	1398	CB	ARG	392	0.212	18.620	55.016	0.50	19.22	AC1
	ATOM	1399	CG	ARG	392	0.060	17.123	55.382	0.50	18.74	AC1
	ATOM	1400	CD	ARG	392	-0.380	16.857	56.840	0.50	19.04	AC1
	ATOM	1401	NE	ARG	392	0.710	17.001	57.811	0.50	18.30	AC1
	ATOM	1402	CZ	ARG	392	0.739	16.427	59.020	0.50	18.32	AC1
10	ATOM	1403	NH1	ARG	392	-0.262	15.660	59.432	0.50	18.09	AC1
	ATOM	1404	NH2	ARG	392	1.783	16.606	59.826	0.50	13.08	AC1
	ATOM	1405	C	ARG	392	0.259	17.833	52.624	0.50	19.79	AC1
	ATOM	1406	O	ARG	392	0.768	16.730	52.453	0.50	19.90	AC1
15	ATOM	1407	N	GLU	393	-0.839	18.220	51.976	1.00	19.51	
	ATOM	1408	CA	GLU	393	-1.484	17.355	50.979	1.00	21.32	
	ATOM	1409	CB	GLU	393	-2.858	17.922	50.575	1.00	23.83	
	ATOM	1410	CG	GLU	393	-3.631	17.066	49.588	1.00	29.44	
	ATOM	1411	CD	GLU	393	-4.209	15.767	50.173	1.00	34.23	
	ATOM	1412	OE1	GLU	393	-3.940	15.434	51.348	1.00	34.71	
	ATOM	1413	OE2	GLU	393	-4.952	15.071	49.433	1.00	37.12	
20	ATOM	1414	C	GLU	393	-0.556	17.210	49.763	1.00	21.12	
	ATOM	1415	O	GLU	393	-0.486	16.147	49.157	1.00	20.35	
	ATOM	1416	N	LYS	394	0.143	18.287	49.395	1.00	19.98	
	ATOM	1417	CA	LYS	394	1.102	18.186	48.302	1.00	21.24	
25	ATOM	1418	CB	LYS	394	1.787	19.519	48.048	1.00	22.05	
	ATOM	1419	CG	LYS	394	0.903	20.468	47.258	1.00	24.02	
	ATOM	1420	CD	LYS	394	1.608	21.778	46.964	1.00	25.62	
	ATOM	1421	CE	LYS	394	0.690	22.711	46.199	1.00	28.47	
30	ATOM	1422	NZ	LYS	394	1.369	24.012	45.959	1.00	30.41	
	ATOM	1423	C	LYS	394	2.153	17.137	48.667	1.00	22.08	
	ATOM	1424	O	LYS	394	2.555	16.341	47.825	1.00	20.82	
	ATOM	1425	N	MET	395	2.590	17.136	49.932	1.00	21.43	
	ATOM	1426	CA	MET	395	3.607	16.166	50.369	1.00	21.13	
35	ATOM	1427	CB	MET	395	4.177	16.520	51.746	1.00	24.05	
	ATOM	1428	CG	MET	395	5.100	17.680	51.738	1.00	24.66	
	ATOM	1429	SD	MET	395	6.457	17.503	50.571	1.00	27.36	
	ATOM	1430	CE	MET	395	6.985	15.797	50.738	1.00	23.91	

	ATOM	1431	C	MET	395	3.121	14.744	50.417	1.00	20.46
	ATOM	1432	O	MET	395	3.872	13.832	50.095	1.00	22.42
	ATOM	1433	N	PHE	396	1.862	14.542	50.827	1.00	20.87
	ATOM	1434	CA	PHE	396	1.285	13.202	50.858	1.00	21.65
5	ATOM	1435	CB	PHE	396	-0.176	13.203	51.374	1.00	20.90
	ATOM	1436	CG	PHE	396	-0.320	13.286	52.875	1.00	22.60
	ATOM	1437	CD1	PHE	396	0.733	12.996	53.727	1.00	22.79
	ATOM	1438	CD2	PHE	396	-1.544	13.640	53.436	1.00	23.58
	ATOM	1439	CE1	PHE	396	0.570	13.063	55.116	1.00	20.29
10	ATOM	1440	CE2	PHE	396	-1.712	13.702	54.826	1.00	23.72
	ATOM	1441	CZ	PHE	396	-0.655	13.416	55.669	1.00	22.24
	ATOM	1442	C	PHE	396	1.281	12.652	49.429	1.00	22.43
	ATOM	1443	O	PHE	396	1.635	11.494	49.215	1.00	21.80
	ATOM	1444	N	LEU	397	0.844	13.462	48.458	1.00	22.96
15	ATOM	1445	CA	LEU	397	0.813	13.022	47.061	1.00	21.97
	ATOM	1446	CB	LEU	397	0.139	14.099	46.176	1.00	22.88
	ATOM	1447	CG	LEU	397	-1.385	14.161	46.354	1.00	23.93
	ATOM	1448	CD1	LEU	397	-1.981	15.078	45.315	1.00	25.27
	ATOM	1449	CD2	LEU	397	-1.972	12.759	46.190	1.00	25.99
20	ATOM	1450	C	LEU	397	2.233	12.705	46.560	1.00	24.94
	ATOM	1451	O	LEU	397	2.450	11.692	45.873	1.00	25.61
	ATOM	1452	N	CYS	398	3.195	13.548	46.924	1.00	23.80
	ATOM	1453	CA	CYS	398	4.593	13.333	46.519	1.00	26.51
	ATOM	1454	CB	CYS	398	5.509	14.454	47.041	1.00	28.87
25	ATOM	1455	SG	CYS	398	5.551	15.910	46.032	1.00	39.48
	ATOM	1456	C	CYS	398	5.111	12.027	47.090	1.00	25.35
	ATOM	1457	O	CYS	398	5.738	11.221	46.399	1.00	25.03
	ATOM	1458	N	LEU	399	4.861	11.821	48.371	1.00	24.81
	ATOM	1459	CA	LEU	399	5.366	10.620	49.009	1.00	24.04
30	ATOM	1460	CB	LEU	399	5.232	10.739	50.530	1.00	24.26
	ATOM	1461	CG	LEU	399	5.806	9.580	51.344	1.00	24.01
	ATOM	1462	CD1	LEU	399	7.281	9.343	50.985	1.00	22.08
	ATOM	1463	CD2	LEU	399	5.672	9.931	52.821	1.00	22.85
	ATOM	1464	C	LEU	399	4.715	9.352	48.518	1.00	26.35
35	ATOM	1465	O	LEU	399	5.398	8.363	48.267	1.00	25.02
	ATOM	1466	N	ASP	400	3.391	9.377	48.361	1.00	27.30

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	ATOM	1467	CA	ASP	400	2.680	8.200	47.874	1.00	29.09
	ATOM	1468	CB	ASP	400	1.179	8.490	47.772	1.00	31.25
	ATOM	1469	CG	ASP	400	0.379	7.258	47.400	1.00	34.75
	ATOM	1470	OD1	ASP	400	0.236	6.356	48.252	1.00	35.16
5	ATOM	1471	OD2	ASP	400	-0.091	7.188	46.250	1.00	38.49
	ATOM	1472	C	ASP	400	3.217	7.816	46.497	1.00	28.91
	ATOM	1473	O	ASP	400	3.436	6.642	46.212	1.00	29.66
	ATOM	1474	N	GLU	401	3.420	8.813	45.644	1.00	28.16
	ATOM	1475	CA	GLU	401	3.936	8.577	44.299	1.00	29.87
10	ATOM	1476	CB	GLU	401	4.052	9.895	43.533	1.00	32.50
	ATOM	1477	CG	GLU	401	4.735	9.751	42.180	1.00	38.83
	ATOM	1478	CD	GLU	401	4.784	11.048	41.406	1.00	42.93
	ATOM	1479	OE1	GLU	401	5.449	12.003	41.865	1.00	45.46
	ATOM	1480	OE2	GLU	401	4.147	11.114	40.334	1.00	45.87
15	ATOM	1481	C	GLU	401	5.308	7.911	44.360	1.00	31.19
	ATOM	1482	O	GLU	401	5.574	6.926	43.650	1.00	31.37
	ATOM	1483	N	TYR	402	6.171	8.444	45.224	1.00	28.55
	ATOM	1484	CA	TYR	402	7.516	7.918	45.365	1.00	29.01
	ATOM	1485	CB	TYR	402	8.314	8.737	46.384	1.00	27.40
20	ATOM	1486	CG	TYR	402	9.667	8.134	46.659	1.00	27.45
	ATOM	1487	CD1	TYR	402	9.849	7.238	47.709	1.00	27.18
	ATOM	1488	CE1	TYR	402	11.087	6.635	47.933	1.00	28.15
	ATOM	1489	CD2	TYR	402	10.747	8.419	45.834	1.00	27.22
	ATOM	1490	CE2	TYR	402	11.996	7.820	46.050	1.00	30.03
25	ATOM	1491	CZ	TYR	402	12.147	6.936	47.097	1.00	30.78
	ATOM	1492	OH	TYR	402	13.374	6.358	47.316	1.00	31.66
	ATOM	1493	C	TYR	402	7.503	6.453	45.769	1.00	30.16
	ATOM	1494	O	TYR	402	8.206	5.641	45.187	1.00	29.67
	ATOM	1495	N	CYS	403	6.700	6.113	46.763	1.00	30.42
30	ATOM	1496	CA	CYS	403	6.616	4.739	47.215	1.00	34.32
	ATOM	1497	CB	CYS	403	5.691	4.650	48.430	1.00	33.37
	ATOM	1498	SG	CYS	403	6.357	5.485	49.920	1.00	31.63
	ATOM	1499	C	CYS	403	6.116	3.820	46.104	1.00	36.81
	ATOM	1500	O	CYS	403	6.612	2.703	45.936	1.00	36.95
35	ATOM	1501	N	ARG	404	5.140	4.289	45.335	1.00	39.50
	ATOM	1502	CA	ARG	404	4.597	3.453	44.271	1.00	42.67

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	ATOM	1503	CB	ARG	404	3.280	4.045	43.746	1.00	43.44
	ATOM	1504	CG	ARG	404	2.135	3.802	44.718	1.00	46.08
	ATOM	1505	CD	ARG	404	0.746	4.164	44.188	1.00	46.89
	ATOM	1506	NE	ARG	404	0.490	5.602	44.159	1.00	46.69
5	ATOM	1507	CZ	ARG	404	0.733	6.386	43.116	1.00	47.48
	ATOM	1508	NH1	ARG	404	1.241	5.874	42.002	1.00	48.94
	ATOM	1509	NH2	ARG	404	0.462	7.684	43.181	1.00	48.22
	ATOM	1510	C	ARG	404	5.578	3.206	43.137	1.00	43.67
	ATOM	1511	O	ARG	404	5.640	2.102	42.598	1.00	44.97
10	ATOM	1512	N	ARG	405	6.356	4.220	42.785	1.00	45.45
	ATOM	1513	CA	ARG	405	7.330	4.098	41.710	1.00	47.72
	ATOM	1514	CB	ARG	405	7.700	5.481	41.167	1.00	49.80
	ATOM	1515	CG	ARG	405	6.535	6.298	40.624	1.00	53.09
	ATOM	1516	CD	ARG	405	7.005	7.695	40.233	1.00	56.62
15	ATOM	1517	NE	ARG	405	5.931	8.506	39.661	1.00	59.35
	ATOM	1518	CZ	ARG	405	5.356	8.263	38.488	1.00	60.20
	ATOM	1519	NH1	ARG	405	5.753	7.231	37.756	1.00	61.80
	ATOM	1520	NH2	ARG	405	4.382	9.049	38.046	1.00	60.75
	ATOM	1521	C	ARG	405	8.609	3.410	42.166	1.00	48.23
20	ATOM	1522	O	ARG	405	9.078	2.464	41.528	1.00	48.90
	ATOM	1523	N	SER	406	9.163	3.891	43.278	1.00	47.66
	ATOM	1524	CA	SER	406	10.421	3.382	43.819	1.00	48.66
	ATOM	1525	CB	SER	406	11.099	4.477	44.638	1.00	49.49
	ATOM	1526	OG	SER	406	11.118	5.698	43.919	1.00	51.64
25	ATOM	1527	C	SER	406	10.336	2.112	44.656	1.00	48.77
	ATOM	1528	O	SER	406	11.355	1.507	44.968	1.00	48.91
	ATOM	1529	N	ARG	407	9.129	1.711	45.026	1.00	49.27
	ATOM	1530	CA	ARG	407	8.948	0.500	45.813	1.00	50.47
	ATOM	1531	CB	ARG	407	9.106	0.811	47.302	1.00	52.25
30	ATOM	1532	CG	ARG	407	10.476	0.434	47.849	1.00	54.88
	ATOM	1533	CD	ARG	407	10.942	1.401	48.918	1.00	55.39
	ATOM	1534	NE	ARG	407	12.157	0.927	49.573	1.00	56.11
	ATOM	1535	CZ	ARG	407	12.885	1.653	50.416	1.00	56.40
	ATOM	1536	NH1	ARG	407	12.524	2.895	50.707	1.00	56.21
35	ATOM	1537	NH2	ARG	407	13.973	1.133	50.972	1.00	55.90
	ATOM	1538	C	ARG	407	7.586	-0.110	45.535	1.00	50.00

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	ATOM	1539	O	ARG	407	6.847	-0.468	46.451	1.00	50.06
	ATOM	1540	N	SER	408	7.279	-0.233	44.248	1.00	49.76
	ATOM	1541	CA	SER	408	6.010	-0.777	43.782	1.00	49.98
	ATOM	1542	CB	SER	408	6.060	-0.957	42.262	1.00	50.23
5	ATOM	1543	OG	SER	408	7.129	-1.806	41.880	1.00	50.48
	ATOM	1544	C	SER	408	5.622	-2.100	44.439	1.00	49.86
	ATOM	1545	O	SER	408	4.444	-2.354	44.698	1.00	50.10
	ATOM	1546	N	SER	409	6.620	-2.933	44.706	1.00	50.01
	ATOM	1547	CA	SER	409	6.412	-4.245	45.307	1.00	49.71
10	ATOM	1548	CB	SER	409	7.704	-5.055	45.217	1.00	50.85
	ATOM	1549	OG	SER	409	8.799	-4.306	45.730	1.00	52.55
	ATOM	1550	C	SER	409	5.954	-4.195	46.758	1.00	49.15
	ATOM	1551	O	SER	409	5.476	-5.195	47.300	1.00	48.48
	ATOM	1552	N	GLU	410	6.095	-3.035	47.392	1.00	47.66
15	ATOM	1553	CA	GLU	410	5.701	-2.912	48.785	1.00	45.50
	ATOM	1554	CB	GLU	410	6.787	-2.197	49.577	1.00	46.29
	ATOM	1555	CG	GLU	410	8.079	-2.980	49.712	1.00	47.76
	ATOM	1556	CD	GLU	410	9.074	-2.261	50.592	1.00	48.13
	ATOM	1557	OE1	GLU	410	10.155	-1.882	50.092	1.00	49.66
20	ATOM	1558	OE2	GLU	410	8.761	-2.063	51.784	1.00	48.57
	ATOM	1559	C	GLU	410	4.373	-2.197	48.973	1.00	44.10
	ATOM	1560	O	GLU	410	4.311	-0.974	49.114	1.00	41.70
	ATOM	1561	N	GLU	411	3.306	-2.985	48.986	1.00	42.76
	ATOM	1562	CA	GLU	411	1.973	-2.451	49.154	1.00	41.57
25	ATOM	1563	CB	GLU	411	0.945	-3.529	48.814	1.00	44.42
	ATOM	1564	CG	GLU	411	1.166	-4.132	47.439	1.00	48.49
	ATOM	1565	CD	GLU	411	0.151	-5.191	47.100	1.00	49.60
	ATOM	1566	OE1	GLU	411	0.111	-6.226	47.806	1.00	49.80
	ATOM	1567	OE2	GLU	411	-0.605	-4.979	46.129	1.00	50.58
30	ATOM	1568	C	GLU	411	1.805	-2.000	50.594	1.00	38.78
	ATOM	1569	O	GLU	411	2.254	-2.682	51.526	1.00	38.53
	ATOM	1570	N	GLY	412	1.170	-0.845	50.768	1.00	34.78
	ATOM	1571	CA	GLY	412	0.953	-0.313	52.103	1.00	32.19
	ATOM	1572	C	GLY	412	2.163	0.402	52.695	1.00	29.28
35	ATOM	1573	O	GLY	412	2.133	0.770	53.865	1.00	28.68
	ATOM	1574	N	ARG	413	3.207	0.625	51.901	1.00	28.70

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	ATOM	1575	CA	ARG	413	4.413	1.286	52.407	1.00	27.65
	ATOM	1576	CB	ARG	413	5.513	1.319	51.348	1.00	29.50
	ATOM	1577	CG	ARG	413	6.850	1.839	51.905	1.00	29.56
	ATOM	1578	CD	ARG	413	8.004	1.721	50.903	1.00	32.68
5	ATOM	1579	NE	ARG	413	9.242	2.244	51.484	1.00	34.48
	ATOM	1580	CZ	ARG	413	9.951	1.632	52.433	1.00	35.49
	ATOM	1581	NH1	ARG	413	9.569	0.454	52.914	1.00	34.87
	ATOM	1582	NH2	ARG	413	11.036	2.221	52.929	1.00	35.73
	ATOM	1583	C	ARG	413	4.153	2.715	52.874	1.00	27.61
10	ATOM	1584	O	ARG	413	4.656	3.142	53.911	1.00	26.64
	ATOM	1585	N	PHE	414	3.377	3.447	52.091	1.00	27.23
	ATOM	1586	CA	PHE	414	3.025	4.829	52.406	1.00	25.72
	ATOM	1587	CB	PHE	414	2.109	5.368	51.290	1.00	27.69
	ATOM	1588	CG	PHE	414	1.553	6.756	51.552	1.00	26.95
15	ATOM	1589	CD1	PHE	414	2.359	7.882	51.454	1.00	28.43
	ATOM	1590	CD2	PHE	414	0.217	6.921	51.891	1.00	29.19
	ATOM	1591	CE1	PHE	414	1.842	9.165	51.692	1.00	28.49
	ATOM	1592	CE2	PHE	414	-0.315	8.199	52.134	1.00	29.46
	ATOM	1593	CZ	PHE	414	0.503	9.325	52.033	1.00	28.75
20	ATOM	1594	C	PHE	414	2.336	4.891	53.777	1.00	26.40
	ATOM	1595	O	PHE	414	2.691	5.702	54.637	1.00	26.65
	ATOM	1596	N	ALA	415	1.355	4.027	53.997	1.00	25.07
	ATOM	1597	CA	ALA	415	0.652	4.002	55.271	1.00	24.63
	ATOM	1598	CB	ALA	415	-0.531	3.028	55.193	1.00	23.72
25	ATOM	1599	C	ALA	415	1.572	3.622	56.436	1.00	24.02
	ATOM	1600	O	ALA	415	1.433	4.142	57.547	1.00	23.15
	ATOM	1601	N	ALA	416	2.518	2.722	56.174	1.00	24.35
	ATOM	1602	CA	ALA	416	3.448	2.270	57.205	1.00	24.54
	ATOM	1603	CB	ALA	416	4.313	1.143	56.666	1.00	24.42
30	ATOM	1604	C	ALA	416	4.319	3.436	57.639	1.00	23.97
	ATOM	1605	O	ALA	416	4.544	3.646	58.832	1.00	25.89
	ATOM	1606	N	LEU	417	4.799	4.192	56.664	1.00	23.99
	ATOM	1607	CA	LEU	417	5.638	5.348	56.952	1.00	23.65
	ATOM	1608	CB	LEU	417	6.056	6.013	55.651	1.00	23.88
35	ATOM	1609	CG	LEU	417	6.940	5.132	54.768	1.00	22.81
	ATOM	1610	CD1	LEU	417	7.104	5.745	53.381	1.00	25.97

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	ATOM	1611	CD2 LEU	417	8.313	4.978	55.464	1.00	24.86
	ATOM	1612	C LEU	417	4.894	6.346	57.843	1.00	23.64
	ATOM	1613	O LEU	417	5.434	6.825	58.851	1.00	24.26
	ATOM	1614	N LEU	418	3.635	6.632	57.517	1.00	22.96
5	ATOM	1615	CA LEU	418	2.896	7.617	58.305	1.00	22.78
	ATOM	1616	CB LEU	418	1.555	7.961	57.622	1.00	22.19
	ATOM	1617	CG LEU	418	1.632	8.536	56.193	1.00	22.93
	ATOM	1618	CD1 LEU	418	0.232	8.983	55.715	1.00	23.88
	ATOM	1619	CD2 LEU	418	2.554	9.749	56.179	1.00	23.65
10	ATOM	1620	C LEU	418	2.646	7.201	59.762	1.00	24.12
	ATOM	1621	O LEU	418	2.372	8.046	60.620	1.00	22.61
	ATOM	1622	N LEU	419	2.706	5.901	60.049	1.00	25.06
	ATOM	1623	CA LEU	419	2.496	5.440	61.404	1.00	27.92
	ATOM	1624	CB LEU	419	2.406	3.909	61.451	1.00	31.65
15	ATOM	1625	CG LEU	419	1.114	3.343	60.884	1.00	34.11
	ATOM	1626	CD1 LEU	419	1.026	1.848	61.218	1.00	36.06
	ATOM	1627	CD2 LEU	419	-0.068	4.081	61.480	1.00	34.83
	ATOM	1628	C LEU	419	3.594	5.891	62.360	1.00	29.85
	ATOM	1629	O LEU	419	3.400	5.885	63.574	1.00	31.55
20	ATOM	1630	N ARG	420	4.736	6.296	61.828	1.00	31.33
	ATOM	1631	CA ARG	420	5.801	6.725	62.718	1.00	31.87
	ATOM	1632	CB ARG	420	7.145	6.755	61.985	1.00	32.74
	ATOM	1633	CG ARG	420	7.648	5.387	61.490	1.00	33.67
	ATOM	1634	CD ARG	420	7.856	4.364	62.622	1.00	36.93
25	ATOM	1635	NE ARG	420	6.709	3.481	62.820	1.00	35.35
	ATOM	1636	CZ ARG	420	6.179	3.194	64.003	1.00	37.82
	ATOM	1637	NH1 ARG	420	6.692	3.714	65.116	1.00	39.26
	ATOM	1638	NH2 ARG	420	5.112	2.408	64.079	1.00	39.04
	ATOM	1639	C ARG	420	5.477	8.092	63.303	1.00	32.15
30	ATOM	1640	O ARG	420	5.995	8.456	64.362	1.00	31.60
	ATOM	1641	N LEU	421	4.591	8.845	62.655	1.00	30.38
	ATOM	1642	CA LEU	421	4.278	10.175	63.164	1.00	29.53
	ATOM	1643	CB LEU	421	3.519	10.976	62.121	1.00	30.72
	ATOM	1644	CG LEU	421	4.322	11.027	60.808	1.00	31.31
35	ATOM	1645	CD1 LEU	421	3.645	12.019	59.885	1.00	32.38
	ATOM	1646	CD2 LEU	421	5.800	11.411	61.053	1.00	31.74

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	ATOM	1647	C	LEU	421	3.582	10.256	64.521	1.00	28.39
	ATOM	1648	O	LEU	421	3.977	11.061	65.363	1.00	26.36
	ATOM	1649	N	PRO	422	2.533	9.446	64.762	1.00	27.69
	ATOM	1650	CD	PRO	422	1.678	8.672	63.839	1.00	27.47
5	ATOM	1651	CA	PRO	422	1.915	9.559	66.090	1.00	26.04
	ATOM	1652	CB	PRO	422	0.717	8.603	66.005	1.00	28.29
	ATOM	1653	CG	PRO	422	0.350	8.664	64.557	1.00	28.91
	ATOM	1654	C	PRO	422	2.906	9.143	67.198	1.00	25.36
	ATOM	1655	O	PRO	422	2.832	9.637	68.322	1.00	24.06
10	ATOM	1656	N	ALA	423	3.821	8.228	66.872	1.00	24.34
	ATOM	1657	CA	ALA	423	4.817	7.779	67.840	1.00	22.88
	ATOM	1658	CB	ALA	423	5.589	6.599	67.273	1.00	26.29
	ATOM	1659	C	ALA	423	5.765	8.942	68.158	1.00	24.20
	ATOM	1660	O	ALA	423	6.094	9.197	69.315	1.00	22.14
15	ATOM	1661	N	LEU	424	6.212	9.640	67.119	1.00	22.92
	ATOM	1662	CA	LEU	424	7.103	10.773	67.309	1.00	22.78
	ATOM	1663	CB	LEU	424	7.512	11.306	65.936	1.00	23.40
	ATOM	1664	CG	LEU	424	8.405	12.531	65.875	1.00	24.54
	ATOM	1665	CD1	LEU	424	9.777	12.226	66.517	1.00	22.52
20	ATOM	1666	CD2	LEU	424	8.589	12.892	64.405	1.00	22.78
	ATOM	1667	C	LEU	424	6.422	11.861	68.153	1.00	22.46
	ATOM	1668	O	LEU	424	7.036	12.468	69.038	1.00	21.68
	ATOM	1669	N	ARG	425	5.136	12.101	67.900	1.00	22.38
	ATOM	1670	CA	ARG	425	4.386	13.095	68.663	1.00	23.67
25	ATOM	1671	CB	ARG	425	2.969	13.240	68.087	1.00	26.56
	ATOM	1672	CG	ARG	425	2.066	14.140	68.903	1.00	30.90
	ATOM	1673	CD	ARG	425	0.977	14.732	68.031	1.00	36.25
	ATOM	1674	NE	ARG	425	0.469	13.774	67.044	1.00	40.86
	ATOM	1675	CZ	ARG	425	-0.070	12.592	67.339	1.00	42.76
30	ATOM	1676	NH1	ARG	425	-0.183	12.196	68.604	1.00	46.63
	ATOM	1677	NH2	ARG	425	-0.498	11.800	66.367	1.00	44.97
	ATOM	1678	C	ARG	425	4.309	12.737	70.150	1.00	21.12
	ATOM	1679	O	ARG	425	4.418	13.604	71.021	1.00	21.30
	ATOM	1680	N	SER	426	4.124	11.452	70.436	1.00	19.60
35	ATOM	1681	CA	SER	426	4.021	10.989	71.820	1.00	19.49
	ATOM	1682	CB	SER	426	3.534	9.539	71.855	1.00	20.63

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	ATOM	1683	OG	SER	426	3.491	9.086	73.198	1.00	23.17	
	ATOM	1684	C	SER	426	5.374	11.096	72.535	1.00	17.38	
	ATOM	1685	O	SER	426	5.458	11.496	73.698	1.00	18.97	
	ATOM	1686	N	ILE	427	6.419	10.742	71.812	1.00	18.11	
5	ATOM	1687	CA	ILE	427	7.770	10.812	72.368	1.00	15.88	
	ATOM	1688	CB	ILE	427	8.763	10.095	71.449	1.00	15.75	
	ATOM	1689	CG2	ILE	427	10.213	10.351	71.913	1.00	17.78	
	ATOM	1690	CG1	ILE	427	8.479	8.591	71.526	1.00	18.23	
	ATOM	1691	CD1	ILE	427	9.082	7.789	70.440	1.00	20.33	
10	ATOM	1692	C	ILE	427	8.146	12.272	72.599	1.00	16.69	
	ATOM	1693	O	ILE	427	8.779	12.589	73.606	1.00	16.41	
	ATOM	1694	N	SER	428	7.767	13.159	71.685	1.00	17.02	
	ATOM	1695	CA	SER	428	8.059	14.590	71.884	1.00	17.37	
	ATOM	1696	CB	SER	428	7.636	15.393	70.633	1.00	18.11	
15	ATOM	1697	OG	SER	428	7.745	16.794	70.876	1.00	19.14	
	ATOM	1698	C	SER	428	7.377	15.138	73.154	1.00	18.08	
	ATOM	1699	O	SER	428	7.968	15.916	73.928	1.00	16.98	
	ATOM	1700	N	LEU	429	6.134	14.741	73.425	1.00	18.84	
	ATOM	1701	CA	LEU	429	5.518	15.249	74.633	1.00	19.23	
20	ATOM	1702	CB	LEU	429	4.054	14.807	74.723	1.00	22.17	
	ATOM	1703	CG	LEU	429	3.187	15.432	73.625	1.00	25.96	
	ATOM	1704	CD1	LEU	429	1.800	14.809	73.624	1.00	28.92	
	ATOM	1705	CD2	LEU	429	3.087	16.943	73.855	1.00	29.57	
	ATOM	1706	C	LEU	429	6.296	14.782	75.860	1.00	17.99	
25	ATOM	1707	O	LEU	429	6.465	15.527	76.816	1.00	18.52	
	ATOM	1708	N	LYS	430	6.778	13.544	75.830	1.00	18.39	
	ATOM	1709	CA	LYS	430	7.540	13.047	76.957	1.00	17.66	
	ATOM	1710	CB	LYS	430	7.780	11.544	76.826	1.00	19.73	
	ATOM	1711	CG	LYS	430	8.539	10.975	78.020	1.00	23.74	
30	ATOM	1712	CD	LYS	430	7.625	11.004	79.260	1.00	27.95	
	ATOM	1713	CE	LYS	430	8.192	10.194	80.414	1.00	34.36	
	ATOM	1714	NZ	LYS	430	7.167	10.122	81.490	1.00	36.64	
	ATOM	1715	C	LYS	430	8.865	13.795	77.077	1.00	18.37	
	ATOM	1716	O	LYS	430	9.346	14.034	78.191	1.00	18.47	
35	ATOM	1717	N	SER	431	9.435	14.174	75.936	0.50	17.09	AC1
	ATOM	1718	CA	SER	431	10.693	14.931	75.919	0.50	18.08	AC1

	ATOM	1719	CB	SER	431	11.102	15.238	74.471	0.50	17.50	AC1
	ATOM	1720	OG	SER	431	12.180	16.159	74.413	0.50	19.63	AC1
	ATOM	1721	C	SER	431	10.472	16.244	76.663	0.50	18.02	AC1
	ATOM	1722	O	SER	431	11.297	16.668	77.464	0.50	17.75	AC1
5	ATOM	1723	N	PHE	432	9.326	16.875	76.415	1.00	17.68	
	ATOM	1724	CA	PHE	432	9.020	18.162	77.057	1.00	17.81	
	ATOM	1725	CB	PHE	432	7.778	18.817	76.425	1.00	18.74	
	ATOM	1726	CG	PHE	432	8.099	19.713	75.249	1.00	17.54	
	ATOM	1727	CD1	PHE	432	8.649	20.976	75.448	1.00	18.72	
10	ATOM	1728	CD2	PHE	432	7.851	19.290	73.958	1.00	17.78	
	ATOM	1729	CE1	PHE	432	8.941	21.800	74.351	1.00	18.20	
	ATOM	1730	CE2	PHE	432	8.135	20.093	72.863	1.00	18.04	
	ATOM	1731	CZ	PHE	432	8.684	21.358	73.060	1.00	19.15	
	ATOM	1732	C	PHE	432	8.817	17.989	78.550	1.00	18.32	
15	ATOM	1733	O	PHE	432	9.170	18.872	79.330	1.00	20.66	
	ATOM	1734	N	GLU	433	8.249	16.852	78.964	1.00	17.15	
	ATOM	1735	CA	GLU	433	8.073	16.592	80.382	1.00	20.50	
	ATOM	1736	CB	GLU	433	7.520	15.192	80.613	1.00	19.84	
	ATOM	1737	CG	GLU	433	6.045	15.053	80.320	1.00	27.71	
20	ATOM	1738	CD	GLU	433	5.533	13.688	80.744	1.00	31.07	
	ATOM	1739	OE1	GLU	433	5.964	13.224	81.823	1.00	34.98	
	ATOM	1740	OE2	GLU	433	4.714	13.094	80.006	1.00	34.76	
	ATOM	1741	C	GLU	433	9.437	16.691	81.052	1.00	19.32	
	ATOM	1742	O	GLU	433	9.574	17.322	82.106	1.00	20.27	
25	ATOM	1743	N	HIS	434	10.438	16.059	80.435	1.00	18.45	
	ATOM	1744	CA	HIS	434	11.810	16.086	80.972	1.00	19.10	
	ATOM	1745	CB	HIS	434	12.708	15.091	80.247	1.00	20.67	
	ATOM	1746	CG	HIS	434	12.346	13.662	80.495	1.00	21.88	
	ATOM	1747	CD2	HIS	434	12.196	12.621	79.642	1.00	22.64	
30	ATOM	1748	ND1	HIS	434	12.153	13.151	81.763	1.00	24.64	
	ATOM	1749	CE1	HIS	434	11.901	11.857	81.678	1.00	26.38	
	ATOM	1750	NE2	HIS	434	11.924	11.509	80.403	1.00	25.49	
	ATOM	1751	C	HIS	434	12.448	17.471	80.900	1.00	19.47	
	ATOM	1752	O	HIS	434	13.029	17.930	81.868	1.00	20.51	
35	ATOM	1753	N	LEU	435	12.360	18.122	79.749	1.00	17.30	
	ATOM	1754	CA	LEU	435	12.926	19.464	79.614	1.00	17.70	

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	ATOM	1755	CB	LEU	435	12.660	20.017	78.219	1.00	17.54
	ATOM	1756	CG	LEU	435	13.350	19.239	77.100	1.00	17.06
	ATOM	1757	CD1	LEU	435	12.933	19.793	75.764	1.00	19.34
	ATOM	1758	CD2	LEU	435	14.874	19.343	77.242	1.00	19.09
5	ATOM	1759	C	LEU	435	12.334	20.411	80.653	1.00	17.96
	ATOM	1760	O	LEU	435	13.034	21.260	81.193	1.00	18.73
	ATOM	1761	N	PHE	436	11.035	20.302	80.921	1.00	17.35
	ATOM	1762	CA	PHE	436	10.460	21.192	81.936	1.00	18.85
	ATOM	1763	CB	PHE	436	8.920	21.188	81.897	1.00	19.91
10	ATOM	1764	CG	PHE	436	8.340	21.916	80.720	1.00	22.43
	ATOM	1765	CD1	PHE	436	8.885	23.113	80.288	1.00	23.77
	ATOM	1766	CD2	PHE	436	7.243	21.399	80.040	1.00	23.20
	ATOM	1767	CE1	PHE	436	8.353	23.783	79.202	1.00	25.60
	ATOM	1768	CE2	PHE	436	6.703	22.063	78.942	1.00	22.41
15	ATOM	1769	CZ	PHE	436	7.250	23.249	78.521	1.00	26.06
	ATOM	1770	C	PHE	436	10.916	20.802	83.332	1.00	20.10
	ATOM	1771	O	PHE	436	11.195	21.670	84.161	1.00	22.89
	ATOM	1772	N	PHE	437	11.001	19.500	83.605	1.00	19.98
	ATOM	1773	CA	PHE	437	11.412	19.023	84.922	1.00	21.11
20	ATOM	1774	CB	PHE	437	11.364	17.484	84.974	1.00	21.57
	ATOM	1775	CG	PHE	437	11.628	16.913	86.339	1.00	25.91
	ATOM	1776	CD1	PHE	437	10.633	16.924	87.313	1.00	27.17
	ATOM	1777	CD2	PHE	437	12.881	16.419	86.665	1.00	27.22
	ATOM	1778	CE1	PHE	437	10.891	16.447	88.599	1.00	30.66
25	ATOM	1779	CE2	PHE	437	13.153	15.942	87.944	1.00	31.40
	ATOM	1780	CZ	PHE	437	12.158	15.957	88.910	1.00	29.78
	ATOM	1781	C	PHE	437	12.807	19.496	85.305	1.00	22.67
	ATOM	1782	O	PHE	437	13.046	19.895	86.464	1.00	24.17
	ATOM	1783	N	PHE	438	13.724	19.453	84.346	1.00	19.58
30	ATOM	1784	CA	PHE	438	15.103	19.888	84.567	1.00	22.15
	ATOM	1785	CB	PHE	438	16.038	19.027	83.718	1.00	22.90
	ATOM	1786	CG	PHE	438	16.093	17.595	84.171	1.00	23.82
	ATOM	1787	CD1	PHE	438	16.725	17.262	85.361	1.00	24.00
	ATOM	1788	CD2	PHE	438	15.509	16.584	83.419	1.00	27.39
35	ATOM	1789	CE1	PHE	438	16.773	15.942	85.795	1.00	25.11
	ATOM	1790	CE2	PHE	438	15.557	15.253	83.847	1.00	27.37

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	ATOM	1791	CZ	PHE	438	16.188	14.935	85.033	1.00	27.90
	ATOM	1792	C	PHE	438	15.334	21.383	84.256	1.00	21.04
	ATOM	1793	O	PHE	438	16.454	21.875	84.352	1.00	22.98
	ATOM	1794	N	HIS	439	14.267	22.077	83.867	1.00	19.84
5	ATOM	1795	CA	HIS	439	14.311	23.503	83.508	1.00	19.79
	ATOM	1796	CB	HIS	439	14.550	24.380	84.742	1.00	21.68
	ATOM	1797	CG	HIS	439	13.463	24.294	85.763	1.00	24.96
	ATOM	1798	CD2	HIS	439	12.345	25.037	85.939	1.00	27.66
	ATOM	1799	ND1	HIS	439	13.440	23.331	86.747	1.00	26.44
10	ATOM	1800	CE1	HIS	439	12.353	23.481	87.481	1.00	27.37
	ATOM	1801	NE2	HIS	439	11.672	24.511	87.012	1.00	28.08
	ATOM	1802	C	HIS	439	15.375	23.803	82.469	1.00	20.93
	ATOM	1803	O	HIS	439	16.185	24.726	82.626	1.00	23.42
	ATOM	1804	N	LEU	440	15.318	23.068	81.366	1.00	16.51
15	ATOM	1805	CA	LEU	440	16.289	23.200	80.301	1.00	18.97
	ATOM	1806	CB	LEU	440	16.820	21.813	79.917	1.00	19.31
	ATOM	1807	CG	LEU	440	17.585	21.101	81.017	1.00	21.82
	ATOM	1808	CD1	LEU	440	17.920	19.672	80.567	1.00	24.43
	ATOM	1809	CD2	LEU	440	18.839	21.874	81.341	1.00	21.97
20	ATOM	1810	C	LEU	440	15.751	23.859	79.042	1.00	20.05
	ATOM	1811	O	LEU	440	16.497	24.030	78.099	1.00	21.82
	ATOM	1812	N	VAL	441	14.478	24.229	79.038	1.00	19.87
	ATOM	1813	CA	VAL	441	13.879	24.814	77.833	1.00	21.84
	ATOM	1814	CB	VAL	441	12.795	23.830	77.247	1.00	22.63
25	ATOM	1815	CG1	VAL	441	11.601	23.713	78.192	1.00	22.79
	ATOM	1816	CG2	VAL	441	12.365	24.276	75.855	1.00	24.87
	ATOM	1817	C	VAL	441	13.306	26.224	78.045	1.00	22.01
	ATOM	1818	O	VAL	441	12.587	26.478	79.009	1.00	20.37
	ATOM	1819	N	ALA	442	13.646	27.122	77.120	1.00	23.96
30	ATOM	1820	CA	ALA	442	13.233	28.529	77.172	1.00	27.08
	ATOM	1821	CB	ALA	442	14.246	29.393	76.392	1.00	28.21
	ATOM	1822	C	ALA	442	11.846	28.718	76.591	1.00	28.96
	ATOM	1823	O	ALA	442	11.655	29.494	75.658	1.00	30.12
	ATOM	1824	N	ASP	443	10.895	28.011	77.178	1.00	30.46
35	ATOM	1825	CA	ASP	443	9.493	27.994	76.764	1.00	31.83
	ATOM	1826	CB	ASP	443	8.678	27.367	77.906	1.00	33.17

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5	ATOM	1827	CG	ASP	443	7.208	27.218	77.581	1.00	34.98
	ATOM	1828	OD1	ASP	443	6.856	26.945	76.404	1.00	37.47
	ATOM	1829	OD2	ASP	443	6.404	27.346	78.524	1.00	31.58
	ATOM	1830	C	ASP	443	8.873	29.320	76.318	1.00	31.97
	ATOM	1831	O	ASP	443	8.426	29.453	75.180	1.00	30.41
10	ATOM	1832	N	THR	444	8.854	30.304	77.205	1.00	32.53
	ATOM	1833	CA	THR	444	8.236	31.586	76.891	1.00	32.98
	ATOM	1834	CB	THR	444	7.965	32.371	78.198	1.00	34.53
	ATOM	1835	OG1	THR	444	9.196	32.581	78.900	1.00	37.04
	ATOM	1836	CG2	THR	444	7.020	31.577	79.102	1.00	35.95
15	ATOM	1837	C	THR	444	8.981	32.486	75.901	1.00	32.99
	ATOM	1838	O	THR	444	8.399	33.436	75.370	1.00	32.71
	ATOM	1839	N	SER	445	10.248	32.179	75.639	1.00	30.56
	ATOM	1840	CA	SER	445	11.071	32.977	74.727	1.00	29.90
	ATOM	1841	CB	SER	445	12.481	33.132	75.313	1.00	29.52
20	ATOM	1842	OG	SER	445	12.418	33.766	76.576	1.00	31.76
	ATOM	1843	C	SER	445	11.199	32.429	73.308	1.00	29.39
	ATOM	1844	O	SER	445	11.580	33.153	72.387	1.00	28.30
	ATOM	1845	N	ILE	446	10.875	31.151	73.133	1.00	26.98
	ATOM	1846	CA	ILE	446	11.010	30.511	71.840	1.00	25.95
25	ATOM	1847	CB	ILE	446	10.656	29.013	71.961	1.00	26.36
	ATOM	1848	CG2	ILE	446	10.295	28.431	70.595	1.00	24.39
	ATOM	1849	CG1	ILE	446	11.864	28.300	72.575	1.00	27.57
	ATOM	1850	CD1	ILE	446	11.637	26.869	72.971	1.00	27.13
	ATOM	1851	C	ILE	446	10.312	31.144	70.640	1.00	25.28
30	ATOM	1852	O	ILE	446	10.917	31.247	69.571	1.00	23.47
	ATOM	1853	N	ALA	447	9.058	31.549	70.809	1.00	26.37
	ATOM	1854	CA	ALA	447	8.316	32.183	69.725	1.00	28.80
	ATOM	1855	CB	ALA	447	6.932	32.606	70.219	1.00	30.52
	ATOM	1856	C	ALA	447	9.114	33.394	69.218	1.00	28.51
35	ATOM	1857	O	ALA	447	9.229	33.608	68.005	1.00	29.41
	ATOM	1858	N	GLY	448	9.675	34.164	70.155	1.00	28.53
	ATOM	1859	CA	GLY	448	10.474	35.337	69.811	1.00	27.89
	ATOM	1860	C	GLY	448	11.762	34.993	69.095	1.00	28.77
	ATOM	1861	O	GLY	448	12.167	35.692	68.162	1.00	28.23
	ATOM	1862	N	TYR	449	12.435	33.927	69.536	1.00	27.26

	ATOM	1863	CA	TYR	449	13.666	33.502	68.872	1.00	28.14
	ATOM	1864	CB	TYR	449	14.262	32.267	69.553	1.00	26.16
	ATOM	1865	CG	TYR	449	14.683	32.492	70.990	1.00	28.82
	ATOM	1866	CD1	TYR	449	14.913	33.782	71.482	1.00	29.84
5	ATOM	1867	CE1	TYR	449	15.336	33.988	72.802	1.00	32.66
	ATOM	1868	CD2	TYR	449	14.881	31.412	71.853	1.00	29.90
	ATOM	1869	CE2	TYR	449	15.306	31.604	73.173	1.00	30.71
	ATOM	1870	CZ	TYR	449	15.532	32.887	73.641	1.00	32.74
	ATOM	1871	OH	TYR	449	15.979	33.070	74.939	1.00	36.98
10	ATOM	1872	C	TYR	449	13.361	33.150	67.420	1.00	27.51
	ATOM	1873	O	TYR	449	14.116	33.491	66.513	1.00	27.99
	ATOM	1874	N	ILE	450	12.254	32.442	67.207	1.00	27.41
	ATOM	1875	CA	ILE	450	11.876	32.053	65.861	1.00	27.70
	ATOM	1876	CB	ILE	450	10.662	31.102	65.863	1.00	26.64
15	ATOM	1877	CG2	ILE	450	10.292	30.744	64.413	1.00	26.88
	ATOM	1878	CG1	ILE	450	11.003	29.846	66.690	1.00	27.46
	ATOM	1879	CD1	ILE	450	9.811	28.956	67.032	1.00	24.45
	ATOM	1880	C	ILE	450	11.534	33.295	65.041	1.00	29.34
	ATOM	1881	O	ILE	450	11.994	33.440	63.911	1.00	30.32
20	ATOM	1882	N	ARG	451	10.735	34.187	65.617	1.00	30.43
	ATOM	1883	CA	ARG	451	10.351	35.416	64.923	1.00	33.00
	ATOM	1884	CB	ARG	451	9.514	36.306	65.851	1.00	32.56
	ATOM	1885	CG	ARG	451	8.874	37.519	65.161	1.00	34.91
	ATOM	1886	CD	ARG	451	7.955	38.328	66.076	1.00	36.14
25	ATOM	1887	NE	ARG	451	6.768	37.599	66.518	1.00	37.46
	ATOM	1888	CZ	ARG	451	6.669	36.943	67.672	1.00	40.02
	ATOM	1889	NH1	ARG	451	7.690	36.921	68.521	1.00	41.16
	ATOM	1890	NH2	ARG	451	5.547	36.299	67.976	1.00	40.59
	ATOM	1891	C	ARG	451	11.629	36.138	64.472	1.00	34.57
30	ATOM	1892	O	ARG	451	11.761	36.516	63.298	1.00	34.59
	ATOM	1893	N	ASP	452	12.578	36.304	65.392	1.00	36.05
	ATOM	1894	CA	ASP	452	13.837	36.975	65.070	1.00	39.88
	ATOM	1895	CB	ASP	452	14.690	37.184	66.331	1.00	42.41
	ATOM	1896	CG	ASP	452	14.004	38.065	67.364	1.00	46.01
35	ATOM	1897	OD1	ASP	452	13.162	38.897	66.961	1.00	46.57
	ATOM	1898	OD2	ASP	452	14.315	37.934	68.576	1.00	48.55

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5	ATOM	1899	C	ASP	452	14.657	36.212	64.039	1.00	40.80
	ATOM	1900	O	ASP	452	15.219	36.805	63.112	1.00	42.52
	ATOM	1901	N	ALA	453	14.730	34.896	64.197	1.00	41.16
	ATOM	1902	CA	ALA	453	15.493	34.071	63.272	1.00	42.41
	ATOM	1903	CB	ALA	453	15.585	32.643	63.796	1.00	41.71
	ATOM	1904	C	ALA	453	14.904	34.070	61.863	1.00	44.06
	ATOM	1905	O	ALA	453	15.635	33.910	60.887	1.00	44.96
10	ATOM	1906	N	LEU	454	13.590	34.259	61.759	1.00	45.34
	ATOM	1907	CA	LEU	454	12.921	34.261	60.460	1.00	47.12
	ATOM	1908	CB	LEU	454	11.419	33.989	60.631	1.00	42.61
	ATOM	1909	CG	LEU	454	11.078	32.514	60.884	1.00	38.89
	ATOM	1910	CD1	LEU	454	9.576	32.329	60.950	1.00	36.29
	ATOM	1911	CD2	LEU	454	11.660	31.657	59.764	1.00	36.23
	ATOM	1912	C	LEU	454	13.149	35.544	59.669	1.00	50.37
15	ATOM	1913	O	LEU	454	13.255	35.506	58.443	1.00	51.61
	ATOM	1914	N	ARG	455	13.218	36.679	60.360	1.00	54.48
	ATOM	1915	CA	ARG	455	13.486	37.951	59.688	1.00	58.31
	ATOM	1916	CB	ARG	455	13.128	39.147	60.582	1.00	59.22
	ATOM	1917	CG	ARG	455	11.635	39.352	60.806	1.00	60.97
	ATOM	1918	CD	ARG	455	11.318	40.787	61.228	1.00	62.50
	ATOM	1919	NE	ARG	455	10.998	40.919	62.648	1.00	64.04
20	ATOM	1920	CZ	ARG	455	11.873	40.784	63.640	1.00	64.71
	ATOM	1921	NH1	ARG	455	13.146	40.511	63.378	1.00	64.92
	ATOM	1922	NH2	ARG	455	11.470	40.923	64.897	1.00	64.48
	ATOM	1923	C	ARG	455	14.988	37.938	59.452	1.00	60.72
	ATOM	1924	O	ARG	455	15.597	38.964	59.147	1.00	61.55
	ATOM	1925	N	ASN	456	15.557	36.743	59.597	1.00	63.01
	ATOM	1926	CA	ASN	456	16.983	36.482	59.463	1.00	64.82
30	ATOM	1927	CB	ASN	456	17.434	36.512	57.987	1.00	66.21
	ATOM	1928	CG	ASN	456	17.254	37.871	57.327	1.00	67.51
	ATOM	1929	OD1	ASN	456	17.901	38.850	57.702	1.00	68.69
	ATOM	1930	ND2	ASN	456	16.377	37.930	56.326	1.00	68.01
	ATOM	1931	C	ASN	456	17.795	37.442	60.317	1.00	65.37
	ATOM	1932	O	ASN	456	17.456	37.680	61.480	1.00	65.63
	ATOM	1933	N	GLY	457	18.858	37.997	59.749	1.00	65.99
35	ATOM	1934	CA	GLY	457	19.704	38.896	60.510	1.00	66.46

	ATOM	1935	C	GLY	457	20.739	38.015	61.176	1.00	66.78
	ATOM	1936	O	GLY	457	21.568	38.471	61.968	1.00	67.21
	ATOM	1937	N	GLY	458	20.669	36.728	60.844	1.00	66.86
	ATOM	1938	CA	GLY	458	21.594	35.753	61.384	1.00	66.84
5	ATOM	1939	C	GLY	458	22.018	34.761	60.315	1.00	66.86
	ATOM	1940	O	GLY	458	21.450	34.801	59.199	1.00	66.65
	ATOM	1941	OXT	GLY	458	22.922	33.943	60.593	1.00	65.49
	ATOM	1942	OH2	TIP	1003	30.252	23.128	74.386	1.00	27.69
	ATOM	1943	OH2	TIP	1005	14.203	25.558	89.644	1.00	25.22
10	ATOM	1944	OH2	TIP	1006	8.388	25.042	72.262	1.00	22.81
	ATOM	1945	OH2	TIP	1008	8.367	21.538	69.460	1.00	19.23
	ATOM	1946	OH2	TIP	1009	-7.350	22.030	52.884	1.00	80.11
	ATOM	1947	OH2	TIP	1010	-4.017	19.644	67.897	1.00	33.26
	ATOM	1948	OH2	TIP	1011	8.365	3.022	77.974	1.00	47.93
15	ATOM	1949	OH2	TIP	1012	30.690	8.779	67.839	1.00	26.30
	ATOM	1950	OH2	TIP	1013	12.264	8.843	80.249	1.00	26.01
	ATOM	1951	OH2	TIP	1014	-1.764	16.382	62.652	1.00	44.82
	ATOM	1952	OH2	TIP	1015	20.301	34.946	75.498	1.00	51.92
	ATOM	1953	OH2	TIP	1016	14.443	15.693	61.296	1.00	22.04
20	ATOM	1954	OH2	TIP	1017	12.487	31.635	78.951	1.00	36.76
	ATOM	1955	OH2	TIP	1018	16.579	6.557	83.739	1.00	27.86
	ATOM	1956	OH2	TIP	1019	-0.626	26.615	50.499	1.00	30.82
	ATOM	1957	OH2	TIP	1021	3.543	20.127	64.859	1.00	23.80
	ATOM	1958	OH2	TIP	1022	4.772	0.996	47.855	1.00	40.67
25	ATOM	1959	OH2	TIP	1023	9.799	29.451	51.621	1.00	30.93
	ATOM	1960	OH2	TIP	1024	7.476	19.030	68.589	1.00	22.30
	ATOM	1961	OH2	TIP	1025	20.355	7.131	58.551	1.00	52.44
	ATOM	1962	OH2	TIP	1026	-0.829	29.526	57.153	1.00	31.90
	ATOM	1963	OH2	TIP	1027	11.560	-6.342	53.442	1.00	52.29
30	ATOM	1964	OH2	TIP	1028	15.278	0.625	72.808	1.00	27.12
	ATOM	1965	OH2	TIP	1029	22.593	26.832	76.012	1.00	35.56
	ATOM	1966	OH2	TIP	1031	3.001	25.878	68.078	1.00	22.76
	ATOM	1967	OH2	TIP	1032	13.489	25.800	47.958	1.00	47.50
	ATOM	1968	OH2	TIP	1033	-7.554	18.088	60.905	1.00	30.53
35	ATOM	1969	OH2	TIP	1034	24.742	18.595	64.446	1.00	44.88
	ATOM	1970	OH2	TIP	1035	13.751	37.059	78.800	1.00	60.77

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	ATOM	1971	OH2 TIP	1036	-0.515	10.167	75.163	1.00	36.51
	ATOM	1972	OH2 TIP	1037	12.373	35.911	72.901	1.00	32.65
	ATOM	1973	OH2 TIP	1039	23.543	26.270	78.523	1.00	24.40
	ATOM	1974	OH2 TIP	1040	17.896	20.961	59.259	1.00	39.57
5	ATOM	1975	OH2 TIP	1041	8.248	15.187	89.930	1.00	59.85
	ATOM	1976	OH2 TIP	1042	7.418	31.128	73.133	1.00	34.33
	ATOM	1977	OH2 TIP	1043	21.123	8.890	53.894	1.00	67.39
	ATOM	1978	OH2 TIP	1045	15.162	18.243	53.355	1.00	28.26
	ATOM	1979	OH2 TIP	1050	4.216	23.224	44.827	1.00	46.56
10	ATOM	1980	OH2 TIP	1051	17.523	1.262	73.909	1.00	23.12
	ATOM	1981	OH2 TIP	1052	-0.169	20.149	67.166	1.00	67.45
	ATOM	1982	OH2 TIP	1053	20.135	12.837	55.866	1.00	51.70
	ATOM	1983	OH2 TIP	1054	10.612	35.387	77.215	1.00	57.20
	ATOM	1984	OH2 TIP	1055	14.587	38.805	73.912	1.00	56.14
15	ATOM	1985	OH2 TIP	1056	22.658	15.094	55.769	1.00	63.46
	ATOM	1986	OH2 TIP	1057	8.196	1.415	39.058	1.00	55.65
	ATOM	1987	OH2 TIP	1058	10.807	2.725	77.173	1.00	22.15
	ATOM	1988	OH2 TIP	1059	19.013	20.604	62.130	1.00	32.43
	ATOM	1989	OH2 TIP	1061	2.388	16.861	45.084	1.00	25.70
20	ATOM	1990	OH2 TIP	1063	5.229	6.816	86.424	1.00	59.99
	ATOM	1991	OH2 TIP	1501	18.919	15.965	66.146	1.00	24.36
	ATOM	1992	OH2 TIP	1502	2.744	33.258	66.246	1.00	30.10
	ATOM	1993	OH2 TIP	1503	4.527	17.244	77.877	1.00	23.98
	ATOM	1994	OH2 TIP	1504	-0.815	22.723	68.903	1.00	24.06
25	ATOM	1995	OH2 TIP	1506	22.697	1.204	69.760	1.00	28.71
	ATOM	1996	OH2 TIP	1507	12.438	25.185	81.547	1.00	28.20
	ATOM	1997	OH2 TIP	1508	17.107	31.275	76.636	1.00	33.34
	ATOM	1998	OH2 TIP	1509	17.900	15.686	59.270	1.00	37.88
	ATOM	1999	OH2 TIP	1510	7.197	12.183	44.002	1.00	29.62
30	ATOM	2000	OH2 TIP	1511	-4.834	15.832	60.463	1.00	33.76
	ATOM	2001	OH2 TIP	1512	11.093	1.186	74.736	1.00	29.08
	ATOM	2002	OH2 TIP	1513	-0.145	2.568	51.845	1.00	30.78
	ATOM	2003	OH2 TIP	1514	-6.100	23.488	73.541	1.00	27.96
	ATOM	2004	OH2 TIP	1515	8.298	14.512	44.198	1.00	34.89
35	ATOM	2005	OH2 TIP	1516	0.418	26.098	68.989	1.00	28.71
	ATOM	2006	OH2 TIP	1517	-7.177	16.116	59.030	1.00	32.04

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	ATOM	2007	OH2 TIP	1519	18.000	18.387	62.314	1.00	32.49
	ATOM	2008	OH2 TIP	1520	21.777	20.403	61.898	1.00	38.66
	ATOM	2009	OH2 TIP	1521	-1.379	32.714	63.883	1.00	40.86
	ATOM	2010	OH2 TIP	1522	1.931	22.610	68.721	1.00	31.49
5	ATOM	2011	OH2 TIP	1523	-3.158	9.157	64.790	1.00	46.08
	ATOM	2012	OH2 TIP	1524	2.081	4.709	65.432	1.00	38.87
	ATOM	2013	OH2 TIP	1525	3.829	11.325	75.940	1.00	34.36
	ATOM	2014	OH2 TIP	1527	21.845	33.747	71.839	1.00	51.86
	ATOM	2015	OH2 TIP	1528	12.196	0.941	78.760	1.00	46.53
10	ATOM	2016	OH2 TIP	1529	30.316	21.478	85.009	1.00	28.49
	ATOM	2017	OH2 TIP	1530	9.786	2.798	91.182	1.00	58.36
	ATOM	2018	OH2 TIP	1531	16.571	8.007	48.772	1.00	38.32
	ATOM	2019	OH2 TIP	1532	3.764	24.595	70.409	1.00	31.40
	ATOM	2020	OH2 TIP	1533	-0.952	5.111	57.996	1.00	39.42
15	ATOM	2021	OH2 TIP	1534	8.395	29.793	48.733	1.00	45.92
	ATOM	2022	OH2 TIP	1535	18.190	-0.943	54.382	1.00	55.57
	ATOM	2023	OH2 TIP	1536	4.583	13.859	64.203	1.00	30.44
	ATOM	2024	OH2 TIP	1538	12.012	14.232	84.365	1.00	33.97
	ATOM	2025	OH2 TIP	1539	-1.284	36.017	69.736	1.00	57.91
20	ATOM	2026	OH2 TIP	1540	2.454	15.898	79.022	1.00	40.22
	ATOM	2027	OH2 TIP	1544	2.719	2.670	49.088	1.00	32.00
	ATOM	2028	OH2 TIP	1545	13.537	37.410	71.136	1.00	41.29
	ATOM	2029	OH2 TIP	1546	22.697	0.071	79.248	1.00	32.01
	ATOM	2030	OH2 TIP	1548	-0.239	7.542	39.851	1.00	52.37
25	ATOM	2031	OH2 TIP	1549	0.076	10.603	44.453	1.00	41.67
	ATOM	2032	OH2 TIP	1550	31.157	3.039	59.611	1.00	43.66
	ATOM	2033	OH2 TIP	1551	4.226	34.045	72.549	1.00	53.58
	ATOM	2034	OH2 TIP	1554	10.022	33.359	56.088	1.00	41.48
	ATOM	2035	OH2 TIP	1555	-1.058	37.708	61.917	1.00	54.81
30	ATOM	2036	OH2 TIP	1556	-4.583	15.870	53.480	1.00	37.02
	ATOM	2037	OH2 TIP	1557	23.851	8.517	92.595	1.00	36.91
	ATOM	2038	OH2 TIP	1558	-7.204	28.744	59.955	1.00	35.72
	ATOM	2039	OH2 TIP	1560	19.483	16.334	88.331	1.00	34.61
	ATOM	2040	OH2 TIP	1561	1.968	8.086	38.648	1.00	57.90
35	ATOM	2041	OH2 TIP	1562	32.430	-4.459	71.625	1.00	63.22
	ATOM	2042	OH2 TIP	1563	7.819	12.682	83.368	1.00	47.71

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	ATOM	2043	OH2 TIP	1564	-5.435	18.376	72.810	1.00	41.90
	ATOM	2044	OH2 TIP	1565	19.550	17.394	63.917	1.00	31.79
	ATOM	2045	OH2 TIP	1566	24.069	28.502	85.703	1.00	50.24
	ATOM	2046	OH2 TIP	1568	26.854	12.830	56.392	1.00	51.68
5	ATOM	2047	OH2 TIP	1570	3.595	32.325	68.760	1.00	45.07
	ATOM	2048	OH2 TIP	1571	24.805	8.300	62.036	1.00	28.27
	ATOM	2049	OH2 TIP	1572	4.194	17.554	63.640	1.00	26.21
	ATOM	2050	OH2 TIP	1573	2.589	20.195	67.352	1.00	34.52
	ATOM	2051	OH2 TIP	1574	15.713	17.937	61.017	1.00	52.03
10	ATOM	2052	OH2 TIP	1575	-9.321	14.210	59.772	1.00	33.92
	ATOM	2053	OH2 TIP	1576	13.215	7.332	82.542	1.00	31.45
	ATOM	2054	OH2 TIP	1577	10.470	24.539	83.194	1.00	35.29
	ATOM	2055	OH2 TIP	1578	25.712	17.999	53.496	1.00	41.46
	ATOM	2056	OH2 TIP	1579	9.445	-0.239	41.882	1.00	41.51
15	ATOM	2057	OH2 TIP	1580	6.603	16.005	42.611	1.00	32.35
	ATOM	2058	OH2 TIP	1581	-1.523	7.654	59.739	1.00	50.11
	ATOM	2059	OH2 TIP	1582	8.397	34.515	72.891	1.00	33.81
	ATOM	2060	OH2 TIP	1583	2.742	39.191	60.949	1.00	39.77
	ATOM	2061	OH2 TIP	1584	18.933	6.009	52.002	1.00	45.27
20	ATOM	2062	OH2 TIP	1585	-1.653	20.171	69.665	1.00	37.15
	ATOM	2063	OH2 TIP	1586	-2.633	4.655	52.475	1.00	49.05
	ATOM	2064	OH2 TIP	1587	36.297	28.180	83.444	1.00	41.56
	ATOM	2065	OH2 TIP	1588	-0.851	31.806	55.808	1.00	34.41
	ATOM	2066	OH2 TIP	1589	4.002	34.625	70.007	1.00	46.13
25	ATOM	2067	OH2 TIP	1590	32.711	20.152	84.581	1.00	53.56
	ATOM	2068	OH2 TIP	1591	19.998	6.099	87.630	1.00	31.12
	ATOM	2069	OH2 TIP	1593	-0.189	3.637	35.682	1.00	54.58
	ATOM	2070	OH2 TIP	1594	12.455	12.705	39.358	1.00	55.12
	ATOM	2071	OH2 TIP	1596	-2.554	-6.074	47.925	1.00	55.01
30	ATOM	2072	OH2 TIP	1597	5.017	28.176	75.017	1.00	42.02
	ATOM	2073	OH2 TIP	1598	28.617	32.433	80.891	1.00	65.40
	ATOM	2074	OH2 TIP	1599	8.680	7.258	78.481	1.00	52.56
	ATOM	2075	OH2 TIP	1600	18.188	12.950	87.437	1.00	47.03
	ATOM	2076	OH2 TIP	1601	-11.532	19.931	55.756	1.00	48.92
35	ATOM	2077	OH2 TIP	1602	22.073	14.215	52.571	1.00	49.32
	ATOM	2078	OH2 TIP	1603	-3.860	34.262	53.170	1.00	48.97

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	ATOM	2079	OH2 TIP	1604	1.118	10.847	82.180	1.00	44.11
	ATOM	2080	OH2 TIP	1605	19.335	32.031	77.782	1.00	48.61
	ATOM	2081	OH2 TIP	1606	19.174	9.955	48.654	1.00	40.42
	ATOM	2082	OH2 TIP	1607	23.632	-1.631	71.300	1.00	37.97
5	ATOM	2083	OH2 TIP	1608	26.622	26.695	85.361	1.00	44.14
	ATOM	2084	OH2 TIP	1609	22.586	-1.769	57.526	1.00	48.15
	ATOM	2085	OH2 TIP	1610	21.977	5.567	60.712	1.00	37.76
	ATOM	2086	OH2 TIP	1611	21.634	2.725	67.903	1.00	41.42
	ATOM	2087	OH2 TIP	1612	4.046	4.187	75.513	1.00	55.86
10	ATOM	2088	OH2 TIP	1614	0.807	25.979	47.960	1.00	38.30
	ATOM	2089	OH2 TIP	1615	17.333	37.351	72.160	1.00	55.70
	ATOM	2090	OH2 TIP	1616	2.475	15.902	62.566	1.00	38.40
	ATOM	2091	OH2 TIP	1618	0.658	14.983	64.592	1.00	60.57
	ATOM	2092	OH2 TIP	1619	-6.509	17.844	52.643	1.00	41.17
15	ATOM	2093	OH2 TIP	1621	27.000	-1.287	80.946	1.00	51.49
	ATOM	2094	OH2 TIP	1622	3.271	9.154	86.392	1.00	55.17
	ATOM	2095	OH2 TIP	1627	3.433	19.409	44.225	1.00	50.54
	ATOM	2096	OH2 TIP	1628	2.390	26.629	72.360	1.00	42.60
	ATOM	2097	OH2 TIP	1629	9.893	39.104	69.833	1.00	54.40
20	ATOM	2098	OH2 TIP	1630	2.709	14.153	43.455	1.00	34.37
	ATOM	2099	OH2 TIP	1631	11.049	12.448	88.232	1.00	45.81
	ATOM	2100	OH2 TIP	1632	4.576	31.506	72.757	1.00	39.34
	ATOM	2101	OH2 TIP	1634	6.784	36.285	71.148	1.00	51.53
	ATOM	2102	OH2 TIP	1635	6.667	43.335	56.568	1.00	51.21
25	ATOM	2103	OH2 TIP	1636	-5.771	9.260	60.442	1.00	44.79
	ATOM	2104	OH2 TIP	1638	0.052	33.418	66.937	1.00	47.03
	ATOM	2105	OH2 TIP	1641	0.354	1.055	46.133	1.00	54.03
	ATOM	2106	OH2 TIP	1642	24.406	30.113	88.300	1.00	48.82
	ATOM	2107	OH2 TIP	1643	26.619	20.182	66.495	1.00	38.01
30	ATOM	2108	OH2 TIP	1644	17.492	7.024	42.815	1.00	65.02
	ATOM	2109	OH2 TIP	1645	25.942	26.481	82.676	1.00	49.52
	ATOM	2110	OH2 TIP	1646	20.601	16.199	68.672	1.00	37.35
	ATOM	2111	OH2 TIP	1649	27.616	9.156	63.460	1.00	37.92
	ATOM	2112	OH2 TIP	1650	0.428	-3.038	44.190	1.00	54.50
35	ATOM	2113	OH2 TIP	1652	-7.028	20.462	59.299	1.00	33.58
	ATOM	2114	OH2 TIP	1653	-2.848	32.314	67.354	1.00	49.02

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	ATOM	2115	OH2 TIP	1654	-0.686	17.762	66.362	1.00	46.03
	ATOM	2116	OH2 TIP	1655	19.583	17.275	60.162	1.00	41.00
	ATOM	2117	OH2 TIP	1656	13.719	36.618	75.139	1.00	51.89
	ATOM	2118	OH2 TIP	1657	9.386	-0.422	71.399	1.00	43.15
5	ATOM	2119	OH2 TIP	1659	23.690	28.880	79.578	1.00	42.62
	ATOM	2120	OH2 TIP	1660	22.069	3.800	58.682	1.00	46.06
	ATOM	2121	OH2 TIP	1661	20.671	13.353	58.841	1.00	57.05
	ATOM	2122	OH2 TIP	1662	27.473	10.135	82.332	1.00	47.43
	ATOM	2123	OH2 TIP	1664	9.564	26.542	84.601	1.00	44.55
10	ATOM	2124	OH2 TIP	1666	29.122	9.606	65.764	1.00	45.20
	ATOM	2125	OH2 TIP	1668	13.135	20.507	41.865	1.00	59.09
	ATOM	2126	OH2 TIP	1669	22.639	11.672	58.999	1.00	54.98
	ATOM	2127	OH2 TIP	1670	-1.845	6.027	76.197	1.00	48.89
	ATOM	2128	OH2 TIP	1672	4.883	25.252	42.734	1.00	51.13
15	ATOM	2129	OH2 TIP	1675	1.329	39.322	66.763	1.00	68.30
	ATOM	2130	OH2 TIP	1676	12.783	29.313	87.079	1.00	54.62
	ATOM	2131	OH2 TIP	1679	25.035	18.339	57.364	1.00	54.53
	ATOM	2132	OH2 TIP	1682	29.392	-1.856	57.721	1.00	37.30
	ATOM	2133	OH2 TIP	1683	28.780	9.970	58.622	1.00	54.22
20	ATOM	2134	OH2 TIP	1685	4.741	39.274	62.499	1.00	46.58
	ATOM	2135	OH2 TIP	1686	-3.084	6.977	49.478	1.00	57.17
	ATOM	2136	OH2 TIP	1687	26.519	30.868	83.197	1.00	64.53
	ATOM	2137	OH2 TIP	1688	-2.784	37.278	67.289	1.00	59.53
	ATOM	2138	OH2 TIP	1689	18.691	10.604	88.296	1.00	52.44
25	ATOM	2139	OH2 TIP	1690	27.919	6.703	82.226	1.00	44.84
	ATOM	2140	OH2 TIP	1691	-4.338	11.103	48.033	1.00	55.91
	ATOM	2141	OH2 TIP	1692	-7.853	9.429	46.864	1.00	63.74
	ATOM	2142	OH2 TIP	1693	10.901	-1.686	67.477	1.00	41.21
	ATOM	2143	OH2 TIP	1694	-2.114	6.315	55.259	1.00	56.21
30	ATOM	2144	OH2 TIP	1695	17.482	15.932	44.391	1.00	41.18
	ATOM	2145	OH2 TIP	1696	-12.326	38.088	61.786	1.00	53.30
	ATOM	2146	OH2 TIP	1697	-2.176	40.471	68.230	1.00	68.88
	ATOM	2147	OH2 TIP	1700	6.514	-1.974	53.366	1.00	51.67
	ATOM	2148	OH2 TIP	1701	21.800	10.610	55.773	1.00	60.93
35	ATOM	2149	OH2 TIP	1702	3.975	27.046	41.446	1.00	44.88
	ATOM	2150	OH2 TIP	1703	26.678	-3.660	64.081	1.00	62.42

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	ATOM	2151	OH2 TIP	1704	2.958	12.027	86.133	1.00	53.52
	ATOM	2152	OH2 TIP	1705	4.264	22.050	63.018	1.00	16.96
	ATOM	2153	OH2 TIP	1706	22.999	26.329	63.006	1.00	32.17
	ATOM	2154	OH2 TIP	1707	5.614	2.688	68.201	1.00	42.08
5	ATOM	2155	OH2 TIP	1708	-2.967	17.730	54.394	1.00	38.89
	ATOM	2156	OH2 TIP	1709	25.853	10.594	62.118	1.00	43.50
	ATOM	2157	OH2 TIP	1711	13.060	12.966	86.563	1.00	41.22
	ATOM	2158	OH2 TIP	1712	19.784	15.472	45.489	1.00	58.17
	ATOM	2159	OH2 TIP	1713	10.567	14.806	42.991	1.00	43.48
10	ATOM	2160	OH2 TIP	1714	24.079	30.190	83.477	1.00	47.61
	ATOM	2161	OH2 TIP	1715	23.927	21.975	63.464	1.00	44.77
	ATOM	2162	OH2 TIP	1716	15.801	20.193	58.769	1.00	34.32
	ATOM	2163	OH2 TIP	1717	23.867	27.717	72.712	1.00	40.47
	ATOM	2164	OH2 TIP	1718	24.567	27.201	69.884	1.00	45.97
15	ATOM	2165	OH2 TIP	1719	32.141	-1.375	73.278	1.00	62.31
	ATOM	2166	OH2 TIP	1720	19.799	24.122	57.454	1.00	35.07
	ATOM	2167	OH2 TIP	1721	18.297	23.286	53.598	1.00	43.88
	ATOM	2168	OH2 TIP	1722	8.617	1.105	73.470	1.00	48.55
	ATOM	2169	OH2 TIP	1723	28.598	25.728	64.296	1.00	46.24
20	ATOM	2170	OH2 TIP	1725	19.225	33.547	73.276	1.00	44.07
	ATOM	2171	OH2 TIP	1726	1.762	4.546	47.584	1.00	50.27
	ATOM	2172	OH2 TIP	1727	10.895	28.774	83.657	1.00	54.87
	ATOM	2173	OH2 TIP	1728	9.989	36.628	73.713	1.00	46.56
	ATOM	2174	OH2 TIP	1729	-1.331	8.332	70.133	1.00	46.76
25	ATOM	2175	OH2 TIP	1730	24.262	12.802	55.386	1.00	59.24
	ATOM	2176	OH2 TIP	1731	28.623	25.788	86.798	1.00	51.87
	ATOM	2177	OH2 TIP	1732	-0.501	4.843	68.521	1.00	47.96
	ATOM	2178	OH2 TIP	1736	18.422	4.635	54.793	1.00	51.00
	ATOM	2179	OH2 TIP	1737	-5.388	27.319	50.727	1.00	46.53
30	ATOM	2180	OH2 TIP	1738	-2.286	20.842	72.915	1.00	45.95
	ATOM	2181	OH2 TIP	1739	0.996	4.268	39.511	1.00	52.67
	ATOM	2182	OH2 TIP	1740	-10.886	28.616	64.116	1.00	45.22
	ATOM	2183	OH2 TIP	1741	20.353	-4.883	70.512	1.00	61.31
	ATOM	2184	OH2 TIP	1742	22.491	16.164	60.365	1.00	58.19
35	ATOM	2185	OH2 TIP	3001	15.272	21.419	87.789	1.00	27.44
	ATOM	2186	OH2 TIP	3002	13.055	32.876	52.925	1.00	53.35

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T00220" 95560660 -

	ATOM	2187	OH2 TIP	3006	16.014	18.841	64.083	1.00	56.45
	ATOM	2188	OH2 TIP	3008	16.802	30.100	54.388	1.00	48.87
	ATOM	2189	OH2 TIP	3009	13.673	27.099	82.740	1.00	32.07
	ATOM	2190	OH2 TIP	3010	30.041	24.325	84.969	1.00	41.40
5	ATOM	2191	OH2 TIP	3007	-2.102	35.612	60.958	1.00	52.05
	ATOM	2192	OH2 TIP	3011	7.242	14.501	40.017	1.00	51.46
	ATOM	2193	OH2 TIP	3012	1.031	36.834	60.593	1.00	49.05
	ATOM	2194	OH2 TIP	3013	0.026	24.244	72.355	1.00	42.35
	ATOM	2195	OH2 TIP	3015	-7.871	31.986	57.037	1.00	46.09
10	ATOM	2196	OH2 TIP	3019	8.655	-3.490	62.423	1.00	44.56
	ATOM	2197	OH2 TIP	3020	-0.191	30.553	51.677	1.00	54.31
	ATOM	2198	OH2 TIP	3023	3.107	37.905	57.599	1.00	48.07
	ATOM	2199	OH2 TIP	3024	26.217	6.182	84.277	1.00	47.75
	ATOM	2200	OH2 TIP	3025	2.594	16.520	65.838	1.00	40.67
15	ATOM	2201	C1 EPH	4000	23.874	12.843	85.264	1.00	42.79
	ATOM	2202	C2 EPH	4000	23.099	13.772	86.129	1.00	44.39
	ATOM	2203	C4 EPH	4000	24.923	13.000	83.062	1.00	45.55
	ATOM	2204	O2 EPH	4000	24.221	13.543	84.059	1.00	44.96
	ATOM	2205	O4 EPH	4000	25.350	11.876	83.028	1.00	47.53
20	ATOM	2206	C18 EPH	4000	25.126	14.045	81.931	1.00	47.05
	ATOM	2207	C19 EPH	4000	24.674	13.569	80.547	1.00	46.98
	ATOM	2208	C20 EPH	4000	23.168	13.412	80.473	1.00	49.00
	ATOM	2209	C21 EPH	4000	22.772	12.939	79.111	1.00	51.06
	ATOM	2210	C22 EPH	4000	21.365	12.327	79.073	1.00	52.88
25	ATOM	2211	C23 EPH	4000	20.291	13.230	78.423	1.00	54.24
	ATOM	2212	C24 EPH	4000	20.651	13.777	77.022	1.00	55.08
	ATOM	2213	C25 EPH	4000	19.987	15.129	76.704	1.00	56.13
	ATOM	2214	C26 EPH	4000	20.807	16.375	77.147	1.00	56.19
	ATOM	2215	C27 EPH	4000	19.981	17.687	77.287	1.00	56.74
30	ATOM	2216	C28 EPH	4000	19.188	18.077	76.015	1.00	56.93
	ATOM	2217	C29 EPH	4000	20.055	18.393	74.792	1.00	57.07
	ATOM	2218	C30 EPH	4000	19.294	18.387	73.442	1.00	58.24
	ATOM	2219	C31 EPH	4000	19.391	17.124	72.550	1.00	58.70
	ATOM	2220	C32 EPH	4000	18.019	16.479	72.198	1.00	59.07
35	ATOM	2221	C33 EPH	4000	16.762	17.158	72.768	1.00	59.61
	ATOM	2222	C34 EPH	4000	15.463	16.541	72.231	1.00	60.17

	ATOM	2223	C37	EPH	4000	22.780	13.059	87.421	1.00	47.03	
	ATOM	2224	O5	EPH	4000	22.047	13.939	88.273	1.00	53.23	
	ATOM	2225	P1	EPH	4000	21.699	13.222	89.578	1.00	56.71	
	ATOM	2226	O6	EPH	4000	20.350	13.536	89.939	1.00	58.07	
5	ATOM	2227	O7	EPH	4000	22.579	12.360	90.311	1.00	56.72	
	ATOM	2228	O8	EPH	4000	22.167	14.340	90.336	1.00	55.93	
	ATOM	2229	C3	EPH	4000	21.561	15.394	85.253	1.00	42.20	
	ATOM	2230	O1	EPH	4000	21.886	14.117	85.454	1.00	40.69	
	ATOM	2231	O3	EPH	4000	22.221	16.347	85.571	1.00	40.97	
10	ATOM	2232	C5	EPH	4000	20.215	15.530	84.546	1.00	40.77	
	ATOM	2233	C6	EPH	4000	20.313	15.776	83.050	1.00	42.19	
	ATOM	2234	C7	EPH	4000	18.924	15.916	82.453	1.00	43.05	
	ATOM	2235	C8	EPH	4000	18.900	15.944	80.947	1.00	44.57	
	ATOM	2236	C9	EPH	4000	17.477	16.101	80.445	1.00	45.49	
15	ATOM	2237	C10	EPH	4000	17.167	15.209	79.273	1.00	47.18	
	ATOM	2238	C11	EPH	4000	16.561	15.987	78.117	1.00	47.85	
	ATOM	2239	C12	EPH	4000	15.158	15.514	77.781	1.00	49.75	
	ATOM	2240	C13	EPH	4000	15.158	14.254	76.932	1.00	49.27	
	ATOM	2241	C14	EPH	4000	14.899	14.563	75.454	1.00	51.41	
20	ATOM	2242	C15	EPH	4000	14.958	13.341	74.490	1.00	51.93	
	ATOM	2243	C16	EPH	4000	16.376	12.870	74.074	1.00	52.39	
	ATOM	2244	C17	EPH	4000	16.681	11.465	74.554	1.00	52.37	
	ATOM	2245	C35	EPH	4000	17.830	11.518	75.525	1.00	52.96	
	ATOM	2246	C36	EPH	4000	17.968	10.168	76.193	1.00	53.00	
25	ATOM	2247	C38	EPH	4000	22.197	10.885	90.057	1.00	56.75	
	ATOM	2248	C39	EPH	4000	23.458	10.026	89.911	1.00	56.42	
	ATOM	2249	N1	EPH	4000	24.546	10.825	89.334	1.00	54.45	
	ATOM	2250	N	SER	236	17.914	25.370	86.674	0.50	20.48	AC2
	ATOM	2251	CA	SER	236	18.176	23.976	86.323	0.50	19.91	AC2
30	ATOM	2252	CB	SER	236	19.157	23.889	85.166	0.50	18.72	AC2
	ATOM	2253	OG	SER	236	19.325	22.538	84.787	0.50	17.70	AC2
	ATOM	2254	C	SER	236	18.741	23.171	87.483	0.50	21.62	AC2
	ATOM	2255	O	SER	236	19.744	23.549	88.075	0.50	20.94	AC2
	ATOM	2256	N	SER	247	25.235	21.608	79.357	0.50	19.68	AC2
35	ATOM	2257	CA	SER	247	25.203	22.865	78.619	0.50	20.48	AC2
	ATOM	2258	CB	SER	247	26.051	23.917	79.337	0.50	19.95	AC2

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	ATOM	2259	OG	SER	247	26.032	25.152	78.637	0.50	20.60	AC2
	ATOM	2260	C	SER	247	25.725	22.638	77.203	0.50	20.84	AC2
	ATOM	2261	O	SER	247	25.203	23.202	76.238	0.50	21.05	AC2
	ATOM	2262	N	SER	271	7.551	30.448	53.176	0.50	29.97	AC2
5	ATOM	2263	CA	SER	271	7.680	31.880	53.442	0.50	31.61	AC2
	ATOM	2264	CB	SER	271	8.888	32.443	52.695	0.50	32.22	AC2
	ATOM	2265	OG	SER	271	8.666	32.395	51.295	0.50	32.71	AC2
	ATOM	2266	C	SER	271	6.432	32.648	53.010	0.50	32.99	AC2
	ATOM	2267	O	SER	271	6.229	33.796	53.408	0.50	34.05	AC2
10	ATOM	2268	N	PRO	319	18.143	-4.099	74.681	0.50	41.20	AC2
	ATOM	2269	CD	PRO	319	18.070	-4.311	76.139	0.50	40.63	AC2
	ATOM	2270	CA	PRO	319	18.053	-2.673	74.356	0.50	38.50	AC2
	ATOM	2271	CB	PRO	319	17.702	-2.038	75.699	0.50	39.26	AC2
	ATOM	2272	CG	PRO	319	18.406	-2.938	76.680	0.50	39.94	AC2
15	ATOM	2273	C	PRO	319	19.321	-2.077	73.756	0.50	35.96	AC2
	ATOM	2274	O	PRO	319	20.410	-2.230	74.313	0.50	35.87	AC2
	ATOM	2275	N	GLN	343	13.913	5.584	80.085	0.50	18.73	AC2
	ATOM	2276	CA	GLN	343	12.714	5.137	79.387	0.50	19.83	AC2
	ATOM	2277	CB	GLN	343	11.463	5.365	80.243	0.50	21.34	AC2
20	ATOM	2278	CG	GLN	343	10.903	4.078	80.837	0.50	26.09	AC2
	ATOM	2279	CD	GLN	343	9.539	4.244	81.488	0.50	27.02	AC2
	ATOM	2280	OE1	GLN	343	9.412	4.823	82.562	0.50	29.15	AC2
	ATOM	2281	NE2	GLN	343	8.508	3.730	80.829	0.50	29.67	AC2
	ATOM	2282	C	GLN	343	12.545	5.813	78.025	0.50	19.53	AC2
25	ATOM	2283	O	GLN	343	12.317	5.141	77.022	0.50	19.10	AC2
	ATOM	2284	N	SER	353	14.027	4.461	65.783	0.50	19.97	AC2
	ATOM	2285	CA	SER	353	15.191	3.950	65.107	0.50	20.43	AC2
	ATOM	2286	CB	SER	353	16.391	4.058	66.033	0.50	20.57	AC2
	ATOM	2287	OG	SER	353	17.540	4.234	65.262	0.50	19.64	AC2
30	ATOM	2288	C	SER	353	15.054	2.524	64.574	0.50	21.08	AC2
	ATOM	2289	O	SER	353	15.234	2.291	63.378	0.50	21.51	AC2
	ATOM	2290	N	ARG	392	0.696	20.186	53.122	0.50	19.50	AC2
	ATOM	2291	CA	ARG	392	0.935	18.822	53.549	0.50	19.96	AC2
	ATOM	2292	CB	ARG	392	0.325	18.551	54.925	0.50	19.99	AC2
35	ATOM	2293	CG	ARG	392	0.603	17.129	55.384	0.50	19.08	AC2
	ATOM	2294	CD	ARG	392	0.140	16.884	56.805	0.50	19.85	AC2

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5 ATOM 2295 NE ARG 392 -1.315 16.885 56.925 0.50 19.23 AC2
ATOM 2296 CZ ARG 392 -1.962 16.577 58.046 0.50 21.63 AC2
ATOM 2297 NH1 ARG 392 -1.283 16.242 59.138 0.50 19.92 AC2
ATOM 2298 NH2 ARG 392 -3.289 16.611 58.086 0.50 22.19 AC2
10 ATOM 2299 C ARG 392 0.338 17.878 52.501 0.50 19.95 AC2
ATOM 2300 O ARG 392 0.940 16.867 52.149 0.50 20.64 AC2
ATOM 2301 N SER 431 9.466 14.172 75.955 0.50 16.96 AC2
ATOM 2302 CA SER 431 10.735 14.900 76.047 0.50 17.25 AC2
ATOM 2303 CB SER 431 11.346 15.109 74.659 0.50 17.09 AC2
10 ATOM 2304 OG SER 431 10.765 16.211 73.998 0.50 16.93 AC2
ATOM 2305 C SER 431 10.466 16.249 76.719 0.50 17.71 AC2
ATOM 2306 O SER 431 11.267 16.716 77.521 0.50 17.14 AC2
END

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Table 2:

bdrxra	----	FNEEMPVEKILDAELAV	----	EPKTEAYME	----
murxra	----	ANEDMPVEKILEAELAV	----	EPKTETYVE	----
rnrxra	----	ANEDMPVEKILEAELAV	----	EPKTETYVE	----
horxra	----	ANEDMPVERILEAELAV	----	EPKTETYVE	----
xlrxra	----	ANEDMPVEKILEAEHAV	----	EPKTETYTE	----
surxrb	-----		-----		-----
aeuspa	----	VRDVTIERIHEAEQLS	----	E	----
dmusp	MTNSVSRDFSIERIIEAEQRA	----	E	----	TQCGDRALTFLR
horxrb	----	APEEMPVDRILEAELAV	----		EQKSDQGVVEGP
murxrb	----	APEEMPVDRILEAELAV	----		EQKSDQGVVEGP
rnrxrb	----	APEEMPVDRILEAELAV	----		EQKSDQGVVEGP
xlrxrbb	----	INEEMPVEKILEAELAV	----		EQKSDQSLE
xlrxrba	----	INEEMPVEKILEAELAV	----		EQKSDQSLE
murxrg	----	SHEDMPVERILEAELAV	----		EPKTESYGD
horxrg	----	GHEDMPVERILEAELAV	----		EPKTESYGD
garxrg	----	GSEDMPVERILEAELAV	----		EPKTEAYS
xlrxrg	----	TSEEMPVERILEAELAV	----		DPKIEAFGD
pmrxr	----	PNDDMPVDKILEAELIS	----		DPKVEQVVP
lmrxr	----	LHTDMPVERILEAEKRV	----	E	----
smrxr	----	TDLPNLTLRCLLSAELSM	----		DPKLAVSERG
amusp	----	LHSDMPIERILEAEKRV	----		ECKMEQQGN
tmusp	----	MQAEMPLDRIIEAEKRI	----		ECTPAGGSG
aarxr	----	GAPPEMPLEIRILEAELRV	----		ESQTGTLS
aarxr2	----	P-GSPDMPLEIRILEAEMRV	----		EQPAPSVLAQ
uprxr	----	AISDMPIASIREAELSV	----		DPIDEQPLDQGVRLQVPLAPPDSEK
cfusp	----	VQVSDLSIERLTEMESLV	----	ADPSEE	----
msusp	----	VQELSIERLLEIESLV	----	ADPPEE	----
bmusp	----	VQELSIERLLELEALV	----	ADSAAE	----
ctusp	----	NGPGRDITVERLMEADQMS	----	EARGCDKS	----
uspx	----	AAAQELSIERLLEMESLVAAAAEE	----	FQFLR	----
rxrmin	----	ASSANEDMPVEKILEAELAV	----	EPKTETYVE	----

bdrxra	-----	SSM	----	SNSTNDPVTNICQAADKQLFTLVEWAKRIPHFS	DL	----	PLDDQVI
murxra	-----	ANMGLNPSSPN	PVTNICQAADKQLFTLVEWAKRIPHFS	SEL	----	PLDDQVI	
rnrxra	-----	ANMGLNPSSPN	PVTNICQAADKQLFTLVEWAKRIPHFS	SEL	----	PLDDQVI	
horxra	-----	ANMGLNPSSPN	PVTNICQAADKQLFTLVEWAKRIPHFS	SEL	----	PLDDQVI	
xlrxra	-----	ANMGLAPNSP	SDPVTNICQAADKQLFTLVEWAKRIPHFS	SDV	----	PLDDQVI	
surxrb	-----	GSGSSPN	PVTNICQAADKQLFTLVEWAKRIPHFS	SSL	----	PLDDQVI	
aeuspa	-----	VGSNSMIPPEYK	GAVSHLCQMVNKQIYQLIDFARRVPHFINL	----	PRDDQVM		
dmusp	-----	VGPYSTVQPDYK	GAVSALCQVVNKQLFQMVVEYARMMPHFAQV	----	PLDDQVI		
horxrb	-----	GATGGGGSSPN	PVTNICQAADKQLFTLVEWAKRIPHFS	SSL	----	PLDDQVI	
murxrb	-----	GATGGGGSSPN	PVTNICQAADKQLFTLVEWAKRIPHFS	SSL	----	PLDDQVI	
rnrxrb	-----	GATGGGGSSPN	PVTNICQAADKQLFTLVEWAKRIPHFS	SSL	----	PLDDQVI	
xlrxrbb	-----	GGGSPSDPVTNICQAADKQLFTLVEWAKRIPHFS	SEL	----	ALDDQVI		
xlrxrba	-----	GGGSPSDPVTNICQDADKQLFTLVEWAKRIPHFS	SELPELPLDDQVI				
murxrg	-----	MNVENSTNDPVTNICHAADKQLFTLVEWAKRIPHFS	SDL	----	TLEDQVI		
horxrg	-----	MNMENSTNDPVTNICHAADKQLFTLVEWAKRIPHFS	SDL	----	TLEDQVI		
garxrg	-----	VNTESSTNDPVTNICHAADKQLFTLVEWAKRIPHFS	SDL	----	TLEDQVI		
xlrxrg	-----	AGLPNSTNDPVTNICHAADKQLFTLVEWAKRIPHFS	SDL	----	PLEDQVI		
pmrxr	-----	FEQVNEENDPVS	NICKAADRQLVTLVEWAKRIPHFS	SSL	----	PLEDQVI	
lmrxr	-----	CKAENQVEYELVEWAKHIPHFTSL	----	PLEDQVL			
smrxr	----	EAIYEDIPGDDDTGLHPLTIICQSIEQQLPRIVNWARQLPVFSSVY	----	LSFDDQFC			
amusp	-----	YENAVSHICNATNKQLFQLVAVAKHIPHFTSL	----	PLEDQVL			
tmusp	-----	GVGEQHDGVNNICQATNKQLFQLVQWAKLIPHFTSL	----	PMSDQVL			
aarxr	-----	AQQQDPVSSICQAADRLHQLVQWAKHIPHFEEL	----	PLEDRMV			
aarxr2	-----	TAASGRDPVNSMCQAAP	PLHELQVQWARRIPHFEEL	----	PIEDRTA		
uprxr	CSFTLPFHPVSEVSCANPLQDVVSNICQAADRLHQLVQWAKHIPHFTDL	----	PIEDQVV				

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bdrxra      LLRAGWNELLIASFSHRSVTVKDG----- ILLATGLHVVH
murxra      LLRAGWNELLIASFSHRSIAVKDG----- ILLATGLHVVH
rnrxra      LLRAGWNELLIASFSHRSIAVKDG----- ILLATGLHVVH
horxra      LLRAGWNELLIASFSHRSIAVKDG----- ILLATGLHVVH
xlrxra      LLRAGWNELLIASFSHRSIAVKDG----- ILLATGLHVVH
surxrb      LLRAGWNELLIASFSHRSIDVRDG----- ILLATGLHVVH
aeuspa      LLRCGWNEMLIAAVAWSMEYIETER----- SSDGSRITVRQPQLMCLGPNFTLH
dmusp       LLKAAWIELLIANVAWCSIVSLDDGGGGGGGLGHDGSFERRSPGLQPQQLFNQSFYSYH
horxrb      LLRAGWNELLIASFSHRSIDVRDG----- ILLATGLHVVH
murxrb      LLRAGWNELLIASFSHRSIDVRDG----- ILLATGLHVVH
rnrxrb      LLRAGWNELLIASFSHRSIDVRDG----- ILLATGLHVVH
xlrxrbb     LLRAGWNELLIASFSHRSISVKDG----- ILLATGLHVVH
xlrxrba     LLRAGWNELLIASFSHRSISEKDG----- ILLATGLHVVH
murxrg      LLRAGWNELLIASFSHRSVSVQDG----- ILLATGLHVVH
horxrg      LLRAGWNELLIASFSHRSVSVQDG----- ILLATGLHVVH
garxrg      LLRAGWNELLIASFSHRSVSVQDG----- ILLATGLHVVH
xlrxrg      LLRAGWNELLIASFSHRSVSVQDG----- ILLATGLHVVH
pmrxr       LLRAGWNELLIASFSHRSIDVKDS----- ILLASGLHVVH
lmrxr       LLRAGWNELLIAAFSHRSVDVKDG----- IVLATGLTVH
smrxr       LIKAAWPELVLISSAYHSTVIRDG----- LLLS IGRHLG
amusp       LLRAGWNELLIASFSHRSIDVKDG----- IVLATGITVH
tmusp       LLRAGWNELLIAAFSHRSIQAQDA----- IVLATGLTVN
aarxr       LLKAGWNELLIAAFSHRSVDVRDG----- IVLATGLVVQ
aarxr2      LLKAGWNELLIAAFSHRSVAVRDG----- IVLATGLVVQ
uprxr       LLKAGWNELLIASFSHRSMGVEDG----- IVLATGLVIH
cfusp       LIKASWNELLFPAIAWRSMEYLEDER----- ENG DGTRSTTQPQLMCLMPGMTLH
msusp       LIKNSWNELLFPAIAWRSMEYLTDER----- ENVD -SRSTAPPQLMCLMPGMTLH
bmusp       LIKGSWNELLFPAIAWRSMEFLNDER----- ENVD -SRNTAPPQLICLMPGMTLH
ctusp       LLKQSLNELLLILNIAYMSIQYVEPDRRNADG----- SLERRQISQQMCLSRNYTLG
uspx        LIKGSWNELLFPAIAWRSMEFLTAAAAA----- PPQLMCLMPGMTLH
rxrmin      LLRAGWNELLIASFSHRSIAVK----- DGILLATGLHVVH
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bdrxra  RSSAHSAGVGSIFDRVLTELVS KM RDMQMDKTELGLCLRAIVLFNPDAGLSNPSEVEALR
murxra  RNSAHSAGVGAI FDRVLTELVS KM RDMQMDKTELGLCLRAIVLFNPD SKGLSNPAEVEALR
rnrxra  RNSAHSAGVGAI FDRVLTELVS KM RDMQMDKTELGLCLRAIVLFNPD SKGLSNPAEVEALR
horxra  RNSAHSAGVGAI FDRVLTELVS KM RDMQMDKTELGLCLRAIVLFNPD SKGLSNPAEVEALR
xlrxra  RNSAHSAGVGAI FDRVLTELVS KM RDMQMDKTELGLCLRAIVLFNPD SKGLSNPLEVEALR
surxrb  RNSAHSAGVGAI FDRVLTELVS KM RDMRMDKTELGLCLRAI ILFNPDAGLSNPSEVEVLR
aeuspa  RNSAQQAGVDTL FDRILCELG I KM RLDVTRAEGLV LKAI ILFNPDIRGLKCQKEIDGMR
dmusp   RNSAIKAGVSAI FDRILSEL SV KM RNLNDRRELSCLKAI ILYNPDIRGIKSRAE IEMCR
horxrb  RNSAHSAGVGAI FDRVLTELVS KM RDMRMDKTELGLCLRAI ILFNPDAGLSNPGEVEILR
murxrb  RNSAHSAGVGAI FDRVLTELVS KM RDMRMDKTELGLCLRAI ILFNPDAGLSNPGEVEILR
rnrxrb  RNSAHSAGVGAI FDRVLTELVS KM RDMRMDKTELGLCLRAI ILFNPDAGLSNPGEVEILR
xlrxrb  RNSAHSAGVGAI FDRVLTELVS KM RDMRMDKTELGLCLRAI ILFNPDAGLSNP GDVEVLR
xlrxrba RNSAHSAGVGAI FERVLTTELVS KM RDMRMDKTELGLCLRAI ILFNPDAGLSNP GDVEVLR
murxrg  RSSAHSRGVGS I FDRVLTELVS KM KDMQMDKSELGCLRAIVLFNPDAGLSNPSEVETLR
horxrg  RSSAHSAGVGS I FDRVLTELVS KM KDMQMDKSELGCLRAIVLFNPDAGLSNPSEVETLR
garxrg  RSSAHSAGVGS I FDRVLTELVS KM KDMQMDKSELGCLRAIVLFNPDAGLSSPSEVESLR
xlrxrg  RSSAHNAGVGS I FDRVLTELVS KM KDMMDKSELGCLRAIVLFNPDAGLSNAAEVEALR
pmrxr   RHSAHQAGVGPI FDRVLTELVS KM RDMMDKTELGLCLRAIVLFNPDVKNLSDSAHIESLR
lmrxr   RNSAHQAGVGTI FDRVLTEL VAKMREMKMDKTELGCLRSVILFNPEVRGLKSQAQEVELLR
smrxr   REVAKSHGLGPLVDR ILHELVARFDLSLQRTTELALLRAI ILFNPDANGLSSRRHVEAVR
amusp   RNSAQQAGVGTI FDRVLSELVSKMREMKMDRTELGCLRSI ILFNPEVRGLKSIQEVTLR

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tmusp K TSAHAVGVGNIYDRVLSELVNKMKEMKMDKTELGLCLRAIILYNPTCRGIKSVQEVEMLR
 aarxr RHSAHGAGVGAI FDRVLTELVAKMREMMDRTELGLCLLAVVLFNPEAKGLRTPSGGPEG
 aarxr2 RHSAHGAGVGDI FDRVLAELVAKMRDMKMDKTELGLCLRAVVLFPNDAKGLRNATRVEALR
 uprxr RSSAHQAGVGAI FDRVLSELVAKMKEMKIDKTELGLCLRSIVLFNPDAGKLNVCNDVEILR
 cfusp RNSAQAGVGAI FDRVLSELSLKMRTLRMDQAEYVALKAI ILLNPDVKGLKNRQEVVDVLR
 msusp RNSALQAGVGQIFDRVLSELSLKMRTLRMDQAEYVALKAI ILLNPDVKGLKNRQEVVDVLR
 bmsup RNSALQAGVGQIFDRVLSELSLKMRSLRMDQAEYVALKAI ILLNPDVKGLKNRQEVVDVLR
 ctusp RNMAVQAGVVQIFDRILSELSVKMKRDLDATELCLLKSIVVFNPDVRLTDDRKSIDLLR
 uspx RNSALQAGVGQIFDRVLSELSLKMRTLRVDQAEYVALKAI ILLNPDVKGLKNRQEVVDVLR
 rxrmin RNSAHSAGVGAI FDRVLTELVS KM RDMQMDKTELGLCLRAIVLFNPD SKGLSNPAEVEALR
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bdrxra EK VYASLEGYTKHNPDPQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
 murxra EK VYASLEAYCKHKYPEQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
 rnrxra EK VYASLEAYCKHKYPEQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
 horxra EK VYASLEAYCKHKYPEQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
 xlrxra EK VYASLEAYCKQKYPEQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
 surxrb EK VYASLETYCKQKYPEQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
 aeuspa EK IYACLDHCKQHPSEDGRFAQLLLRLPALRSISLKCLDHLNFIIRLLSDKHLDSFIVE
 dmusp EK VYACLDHCRLEHPPGDDGRFAQLLLRLPALRSISLKCLDHLFLFRITSDRPLEELFLE
 horxrb EK VYASLETYCKQKYPEQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
 murxrb EK VYASLETYCKQKYPEQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
 rnrxrb EK VYASLETYCKQKYPEQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
 xlrxbbb EK VYASLESYCKQKYPDQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
 xlrxbba EK VYACLESYCKQKYPDQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
 murxrg EK VYATLEAYTKQKYPEQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
 horxrg EK VYATLEAYTKQKYPEQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
 garxrg EK VYATLEAYTKQKYPEQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
 xlrxrg EK VYATLESYTKQKYPDQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
 pmxr EK VYASLEAYCRSKYPDQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDKFLMN
 lmrxr EK VYAALEEYTRTTHPDEPGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDVPIDTFLME
 smxr EQLYSALHSYCTTNQPDTSRFTKLLRLPLRSIASKCLEHLVFFVLAEDPTSCRLIN
 amusp EK IYGALEGYCRVAVPDDAGRFAKLLRLPAIRSIGLKCLEYLFFFKMIGDVPIDDFLVE
 tmusp EK IYGVLEEYTRTTHPNEPGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDVPIDTFLME
 aarxr ESV - SALEEHCRQYDPDQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDNFLLS
 aarxr2 EK VYAALEEHCRRHHPDQGRFGKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDSFLLN
 uprxr EK VYAALEEYTRTTPDEPGRFAKLLRLPALRSIGLKCLEYLFFLKLIGDTPIDSYLMK
 cfusp EKMFSCLDYCRSRSENEGRFASLLRLPALRSISLKSFHEHYFFHLVAEGSISGYIRE
 msusp EKMFSCLDYVRRSRCAEEGRFAALLRLPALRSISLKCFEHLFFHLVADTSIASYIHD
 bmsup EKMFCLCLDEYCRSRSGEEGRFAALLRLPALRSISLKSFHEHYLFHLVAEGSVSSYIRD
 ctusp SRIYASLDEYCRQKHPNEDGRFAQLLLRLPALRSISLKCLDHLFFYQLIDDKNVENSIVIE
 uspx EKMFCLCLDEYCRSRSEEGRFAALLRLPALRSISLKSFHEHLFFHLVADTSIAGYIRD
 rxrmin EK VYASLEAYCKHKYPEQGRFAKLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
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bdrxra MLEAPHQIT
 murxra MLEAPHQAT
 rnrxra MLEAPHQTT
 horxra MLEAPHQMT
 xlrxra MLEAPHQMT
 surxrb -----
 aeuspa MLDMPI ---
 dmusp QLEAPPPPG
 horxrb MLEAPHQLA
 murxrb MLEAPHQLA
 rnrxrb MLEAPHQLA
 xlrxbbb MLEAPHQLS
 xlrxbba MLEAPHQLS
 murxrg MLETPLQIT
 horxrg MLETPLQIT
 garxrg MLETPLQVT
 xlrxrg MLETPLQIS

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pmrxr	MLETTSDFP
lmrxr	MLESPSDS-
smrxr	LVEHGVWPI
amusp	MLESRSDP-
tmusp	MLESPADA-
aarxr	MLEAPSDP-
aarxr2	MLEAPADP-
uprxr	MLVDNPNTS
cfusp	ALRNHAPPI
msusp	ALRNHAPSI
bmusp	ALCNHAPPI
ctusp	EFHKLN---
uspx	ALRNGG---
rxrmin	MLEAP----

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References

1. Oro A.E. et al. (1990): Relationship between the product of the *Drosophila* ultraspiracle locus and the vertebrate retinoid X receptor. *Nature* 347, 298-301
2. Moras D. & Gronemeyer H. (1998): The nuclear receptor ligand-binding domain: structure and fiction. *Current Opinion in Cell Biology* 10, 384-391
3. Segraves W.A. (1994): Steroid Receptors and Other Transcription Factors in Ecdysone Response. *Recent Progress in Hormone Research*, 49, 167-195
4. Henrich V.C. & Brown N.E. (1995): Insect Nuclear Receptors: A Developmental and Comparative Perspective. *Insect Biochem. Mol. Biol.* 25 (8), 881-897
5. Thummel C.S. (1995): From Embryogenesis to Metamorphosis: The Regulation and Function of *Drosophila* Nuclear Receptor Superfamily Members. *Cell* 83, 871-877
6. Truman J.W. (1996): Ecdysis Control Sheds Another Layer. *Science* 271, 40-41
7. Yao T. et al. (1993): Functional ecdysone receptor is the product of EcR and Ultraspiracle genes. *Nature* 366, 476-479
8. Hall B.L. & Thummel C.S. (1998): The RXR homolog Ultraspiracle is an essential component of the *Drosophila* ecdysone receptor. *Development* 125, 4709-4717
9. Lezzi M. et al. (1999): The Ecdysone Receptor Puzzle. *Arch. Insect Biochem. Physiol.* 41, 99-106
10. Mikitani K. (1996): Ecdysteroid Receptor Binding Activity and Ecdysteroid Agonist Activity at the Level of Gene Expression are Correlated with the Activity of Dibenzoyl Hydrazines in Larvae of *Bombyx mori*. *J. Insect Physiol.* 42 (10), 937-941
11. Dhadialla T.S. et al. (1998): New Insecticides with Ecdysteroidal and Juvenile Hormone Activity. *Annu. Rev. Entomol.* 43, 545-569

12. Sundaram M. et al. (1998): Basis for selective action of a synthetic molting hormone agonist, RH-5992 on lepidopteran insects. *Insect Biochem. Mol. Biol.* 28, 693-704
13. Rarey M. et al. (1996): Predicting Receptor-Ligand Interactions by an Incremental Construction Algorithm. *J. Mol. Biol.* 261(3), 470-489
14. Jones G. et al. (1997): Development and Validation of a Genetic Algorithm for Flexible Docking. *J. Mol. Biol.* 267 (3), 727-748
15. Böhm H.J. (1992): LUDI: Rule-Based Automatic Design of New Substituents for Enzyme Inhibitor Leads. *J. Comp.-Aided Mol. Design* 6, 593-606
16. Nishibata Y. & Itai A. (1991): Automatic creation of drug candidate structures based on receptor structure. Starting point for artificial lead generation. *Tetrahedron* 47, 8985-8990
17. Moon J.B. & Howe W.J. (1991): Computer design of bioactive molecules: a method for receptor-based de novo ligand design. *Proteins* 11 (4), 314-328
18. Otwinowski Z. & Minor W. (1997): Processing of X-ray diffraction data collected in oscillation mode. *Methods Enzymol.* 276, 307-326
19. Navaza J. (1994): Amore: an automated package for molecular replacement. *Acta Cryst. A* 50, 157-163
20. Egea P.F. et al. (2000): Crystal structure of the human RXRalpha ligand-binding domain bound to its natural ligand 9-cis retinoic acid. *EMBO J.* 19, 2592-2601
21. Jones T.A. et al. (1991): Improved methods for generating protein models in electron density maps and the location of errors in these models. *Acta Cryst. A* 47, 110-119
22. Perrakis A. et al (1997): wARP: improvement and extension of crystallographic phases by weighted averaging of multiple-refined dummy atomic models. *Acta Cryst. D* 53, 448-455
23. Brünger A.T. et al. (1998): Crystallography & NMR System: A New Software Suite for Macromolecular Structure Determination. *Acta Cryst. D* 54, 905-921

24. Laskowski R.A. et al. (1993): PROCHECK:a programme to check the stereochemical quality of protein structure coordinates. J. Appl. Crystallogr. 26, 283-291

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